

Spectral theory of Schrödinger operators with infinitely many point interactions and radial positive definite functions

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Abstract

A number of results on radial positive definite functions on \mathbb{R}^n related to Schoenberg's integral representation theorem are obtained. They are applied to the study of spectral properties of self-adjoint realizations of two- and three-dimensional Schrödinger operators with countably many point interactions. In particular, we find conditions on the configuration of point interactions such that any self-adjoint realization has purely absolutely continuous non-negative spectrum. We also apply some results on Schrödinger operators to obtain new results on completely monotone functions.

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Key words. Schrödinger operator, point interactions, self-adjoint extension, spectrum, positive definite function

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1 Introduction

An important topic in quantum mechanics is the spectral theory of Schrödinger Hamiltonians with point interactions. These are Schrödinger operators on the Hilbert space $L^2(\mathbb{R}^d)$, $1 \leq d \leq 3$, with potentials supported on a discrete (finite or countable) set of points of \mathbb{R}^d . There is an extensive literature on such operators, see e.g. [4, 6, 10, 21, 23, 28, 29, 30, 32, 45] and references therein.

Let $X = \{x_j\}_1^m$ be the set of points in \mathbb{R}^d and let $\alpha = \{\alpha_j\}_1^m$ be a sequence of real numbers, where $m \in \mathbb{N} \cup \{\infty\}$. The mathematical problem is to associate a self-adjoint operator (Hamiltonian) on $L^2(\mathbb{R}^d)$ with the differential expression

$$\mathfrak{L}_d := \mathfrak{L}_d(X, \alpha) := -\Delta + \sum_{j=1}^m \alpha_j \delta(\cdot - x_j), \quad \alpha_j \in \mathbb{R}, \quad m \in \mathbb{N} \cup \{\infty\}, \quad (1.1)$$

and to describe its spectral properties.

There are at least two natural ways to associate a self-adjoint Hamiltonian $H_{X,\alpha}$ with the differential expression (1.1). The first one is the form approach. That is, the Hamiltonian $H_{X,\alpha}$ is defined by the self-adjoint operator associated with the quadratic form

$$\mathfrak{t}_{X,\alpha}^{(d)}[f] = \int_{\mathbb{R}^d} |\nabla f|^2 dx + \sum_{j=1}^m \alpha_j |f(x_j)|^2, \quad \text{dom}(\mathfrak{t}_{X,\alpha}^{(d)}) = W_{\text{comp}}^{2,2}(\mathbb{R}^d). \quad (1.2)$$

This is possible for $d = 1$ and finite $m \in \mathbb{N}$, since in this case *the quadratic form $\mathfrak{t}_{X,\alpha}^{(1)}$ is semibounded below and closable* (cf. [47]). Its closure $\mathfrak{t}_{X,\alpha}^{(1)}$ is defined by the same expression (1.2) on the domain $\text{dom}(\mathfrak{t}_{X,\alpha}^{(1)}) = W^{1,2}(\mathbb{R})$. For $m = \infty$ the form (1.2) is also closable whenever it is semibounded (see [7, Corollary 3.3]).

Another way to introduce local interactions on $X := \{x_j\}_{j=1}^m \subset \mathbb{R}$ is to consider the minimal operator corresponding to the expression \mathfrak{L}_1 and to impose boundary conditions at the points x_j . For instance, in the case $d = 1$ and $m < \infty$ the domain of the corresponding Hamiltonian $H_{X,\alpha}$ is given by

$$\text{dom}(H_{X,\alpha}) = \{f \in W^{2,2}(\mathbb{R} \setminus X) \cap W^{1,2}(\mathbb{R}) : f'(x_j+) - f'(x_j-) = \alpha_j f(x_j)\}.$$

In contrast to the one-dimensional case, the quadratic form (1.2) *is not closable* in $L^2(\mathbb{R}^d)$ for $d \geq 2$, so it does not define a self-adjoint operator. The latter happens because the point evaluations $f \rightarrow f(x)$ are no longer continuous on the Sobolev space $W^{1,2}(\mathbb{R}^d)$ in the case $d \geq 2$.

However, it is still possible to apply the extension theory of symmetric operators. F. Berezin and L. Faddeev proposed in their pioneering paper [10] to consider the expression (1.1) (with $m = 1$ and $d = 3$) in this framework. They defined the minimal symmetric operator H as a restriction of $-\Delta$ to the domain $\text{dom } H = \{f \in W^{2,2}(\mathbb{R}^d) : f(x_1) = 0\}$ and studied the spectral properties of *all its self-adjoint extensions*. Self-adjoint extensions (or realizations) of H for finitely many point interactions have been investigated since then in numerous papers (see [4]). In the case of infinitely many point interactions $X = \{x_j\}_1^\infty$ the minimal operator H_{\min} is defined by

$$H_d := H_{d,\min} := -\Delta \upharpoonright \text{dom } H, \quad \text{dom}(H_d) = \{f \in W^{2,2}(\mathbb{R}^d) : f(x_j) = 0, \quad j \in \mathbb{N}\}. \quad (1.3)$$

In this paper we investigate the "operator" (1.1) (with $d = 3$ and $m = \infty$) in the framework of boundary triplets. This is a new approach to the extension theory of symmetric operators

that has been developed during the last three decades (see [22, 17, 15, 49]). A boundary triplet $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ for the adjoint of a densely defined symmetric operator A consists of an auxiliary Hilbert space \mathcal{H} and two linear mappings $\Gamma_0, \Gamma_1 : \text{dom}(A^*) \rightarrow \mathcal{H}$ such that the mapping $\Gamma := (\Gamma_0, \Gamma_1) : \text{dom}(A^*) \rightarrow \mathcal{H} \oplus \mathcal{H}$ is surjective. The main requirement is the abstract Green identity

$$(A^*f, g)_{\mathfrak{H}} - (f, A^*g)_{\mathfrak{H}} = (\Gamma_1 f, \Gamma_0 g)_{\mathcal{H}} - (\Gamma_0 f, \Gamma_1 g)_{\mathcal{H}}, \quad f, g \in \text{dom}(A^*). \quad (1.4)$$

A boundary triplet for A^* exists whenever A has equal deficiency indices, but it is not unique. It plays the role of a "coordinate system" for the quotient space $\text{dom}(A^*)/\text{dom}(\overline{A})$ and leads to a natural parametrization of the self-adjoint extensions of A by means of self-adjoint linear relations (multi-valued operators) in \mathcal{H} , see [22] and [49] for detailed treatments.

The main analytical tool in this approach is the abstract Weyl function $M(\cdot)$ which was introduced and studied in [17]. This Weyl function plays a similar role in the theory of boundary triplets as the classical Weyl-Titchmarsh function does in the theory of Sturm-Liouville operators. In particular, it allows one to investigate spectral properties of extensions (see [13, 17, 38, 41]).

When studying boundary value problems for differential operators, one is searching for an appropriate boundary triplet such that:

- the properties of the mappings $\Gamma = \{\Gamma_0, \Gamma_1\}$ should correlate with trace properties of functions from the maximal domain $\text{dom}(A^*)$,
- the Weyl function and the boundary operator should have "good" explicit forms.

Such a boundary triplet was constructed and applied to differential operators with infinite deficiency indices in the following cases:

- (i) smooth elliptic operators in bounded or unbounded domains ([24], [55], see also [25]),
- (ii) the maximal Sturm-Liouville operator $-d^2/dx^2 + T$ in $L^2([0, 1]; \mathcal{H})$ with an unbounded operator potential $T = T^* \geq aI$, $T \in \mathcal{C}(\mathcal{H})$ ([22], see also [17] for the case of $L^2(\mathbb{R}_+; \mathcal{H})$),
- (iii) the 1D Schrödinger operator $\mathfrak{L}_{1,X}$ in the cases $d_*(X) > 0$ ([33], [43]) and $d_*(X) = 0$ ([34]), where $d_*(X)$ is defined by (1.5) below.

Constructing such a "good" boundary triplet involves always nontrivial analytic results. For instance, Grubb's construction [24] for (i) (see also the adaptation to the case of Definition 4.1 in [39]) is based on trace theory for elliptic operators developed by Lions and Magenes [36] (see also [25]). The approach in (iii) is based on a general construction of a (regularized) boundary triplet for direct sums of symmetric operators (see [41, Theorem 5.3] and [34, Theorem 3.10]).

In this paper we study *all* (that is, not necessarily local) self-adjoint extensions of the operator $H = H_3$ (realizations of \mathfrak{L}_3) in the framework of boundary triplets approach. As in [4] our crucial assumption is

$$d_*(X) := \inf_{j \neq k} |x_k - x_j| > 0. \quad (1.5)$$

Our construction of a boundary triplet Π for H^* is based on the following result: *The sequence*

$$\left\{ \frac{e^{-|x-x_j|}}{|x-x_j|} \right\}_{j=1}^{\infty} \quad (1.6)$$

forms a Riesz basis of the defect subspace $\mathfrak{N}_{-1}(H) = \ker(H^* + I)$ of H^* (cf. Theorem 3.8). Using this boundary triplet Π we parameterize the set of self-adjoint extensions of H , compute the corresponding Weyl function $M(\cdot)$ and investigate various spectral properties of self-adjoint extensions (semi-boundedness, non-negativity, negative spectrum, resolvent comparability, etc.)

Our main result on spectral properties of Hamiltonians with point interactions concerns the absolutely continuous spectrum (*ac*-spectrum). For instance, if

$$C := \sum_{|j-k|>0} \frac{1}{|x_j - x_k|^2} < \infty, \quad (1.7)$$

we prove that the part $\tilde{H}E_{\tilde{H}}(C, \infty)$ of *every self-adjoint extension* \tilde{H} of H is absolutely continuous (cf. Theorems 5.13 and 5.14). Moreover, under additional assumptions on X , we show that the singular part of $\tilde{H}_+ := \tilde{H}E_{\tilde{H}}(0, \infty)$ is trivial, i.e. $\tilde{H}_+ = \tilde{H}_+^{ac}$.

The absolute continuity of self-adjoint realizations \tilde{H} of H has been studied only in very few cases. Assuming that $X = Y + \Lambda$, where $Y = \{y_j\}_1^N \in \mathbb{R}^3$ is a finite set and $\Lambda = \{\sum_1^3 n_j a_j \in \mathbb{R}^3 : (n_1, n_2, n_3) \in \mathbb{Z}^3\}$ is a Bravais lattice, it was proved in [3, 5, 23, 28, 29, 30, 6] (see also [4, Theorems 1.4.5, 1.4.6] and the references in [4] and [6]) that the spectrum of some periodic realizations is absolutely continuous and has a band structure with a finite number of gaps.

An important feature of our investigations is an apparently new *connection between the spectral theory of operators (1.1) for $d = 3$ and the class Φ_3 of radial positive definite functions on \mathbb{R}^3* . We exploit this connection in both directions. In Section 2 we combine the extension theory of the operator H with Theorem 3.8 to obtain results on positive definite functions and the corresponding Gram matrices (1.8), while in Section 5 positive definite functions are applied to the spectral theory of self-adjoint realizations of operators (1.1) with infinitely many point interactions.

The paper consists of two parts and is organized as follows.

Section 2 deals with radial positive definite functions on \mathbb{R}^d and has been inspired by possible applications to the spectral theory of operators (1.1). If f is such a function and $X = \{x_n\}_1^\infty$ is a sequence of points of \mathbb{R}^d , we say that f is *strongly X -positive definite* if there exists a constant $c > 0$ such that for all $\xi_1, \dots, \xi_m \in \mathbb{C}$,

$$\sum_{j,k=1}^m \xi_k \bar{\xi}_j f(x_k - x_j) \geq c \sum_{k=1}^m |\xi_k|^2, \quad m \in \mathbb{N}.$$

Using Schoenberg's theorem we derive a number of results showing under certain assumptions on X that f is strongly X -positive definite and that the Gram matrix

$$Gr_X(f) := (f(|x_k - x_j|))_{k,j \in \mathbb{N}} \quad (1.8)$$

defines a bounded operator on $l^2(\mathbb{N})$. The latter results correlate with the properties of the sequence $\{e^{i(\cdot, x_k)}\}_{k \in \mathbb{N}}$ of exponential functions to form a Riesz-Fischer sequence or a Bessel sequence, respectively, in $L^2(S_r^n; \sigma_n)$ for some $r > 0$.

In Section 3 we prove that the sequence (1.6) forms a Riesz basis in the closure of its linear span if and only if X satisfies (1.5). This result is applied to prove that *for such X and any non-constant absolute monotone function f on \mathbb{R}_+ the function $f(|\cdot|_3)$ is strongly X -positive definite*. Under an additional assumption it is shown that the matrix (1.8) defines a boundedly invertible bounded operator on $l^2(\mathbb{N})$ (see Theorem 2.10).

The second part of the paper is devoted to the spectral theory of self-adjoint operators associated with the expression (1.1) for countably many point interactions. Throughout this part we assume that X satisfies condition (1.5).

In Section 4 we collect some basic definitions and facts on boundary triplets, the corresponding Weyl functions and spectral properties of self-adjoint extensions.

In Subsection 5.1 we construct a boundary triplet for the adjoint operator H^* for $d = 3$ and compute the corresponding Weyl function $M(\cdot)$. The explicit form of the Weyl function given by (5.11) plays crucial role in the sequel. For the proof of the surjectivity of the mapping $\Gamma = (\Gamma_0, \Gamma_1)$ the strong X -positive definiteness of the function $e^{-|\cdot|}$ on \mathbb{R}^3 is essentially used. The latter follows from the absolute monotonicity of the function e^{-t} on \mathbb{R}_+ .

In Subsection 5.2 we describe the quadratic form generated by the semibounded operator $M(0)$ on $l^2(\mathbb{N})$ as strong resolvent limit of the corresponding Weyl function $M(-x)$ as $x \rightarrow +0$. For this we use the strong X -positive definiteness of the function $\frac{1-e^{-|\cdot|}}{|\cdot|}$ on \mathbb{R}^3 which follows from the absolute monotonicity of the function $\frac{1-e^{-t}}{t}$ on \mathbb{R}_+ . The operator $M(0)$ enters into the description of the Krein extension of H for $d = 3$ and allow us to characterize all non-negative self-adjoint extensions as well as all self-adjoint extensions with $\kappa(\leq \infty)$ negative eigenvalues. Using the behaviour of the Weyl function at $-\infty$ we show that any self-adjoint extension H_B of H is semibounded from below if and only if the corresponding boundary operator B is. A similar result for elliptic operators on exterior domains has recently been obtained by G. Grubb [26].

In Subsection 5.3 we apply a technique elaborated in [13, 41] as well as a new general result (Lemma 5.12) to investigate the ac -spectrum of self-adjoint realizations. In particular, we prove that the part $\widetilde{H}E_{\widetilde{H}}(C, \infty)$ of *any self-adjoint realization* \widetilde{H} of \mathfrak{L}_3 is *absolutely continuous* provided that condition (1.7) holds. Moreover, under some additional assumptions on X we show that the singular non-negative part $\widetilde{H}^sE_{\widetilde{H}}(0, \infty)$ of any realization \widetilde{H} is trivial. Among others, Theorems 5.13 and 5.14 provide explicit examples which show that an analog of the Weyl–von Neumann theorem does not hold for non-additive (singular) compact (and even non-compact) perturbations. The proof of these results is based on the fact that the function $\frac{\sin st}{t}$ belongs to Φ_3 for each $s > 0$. Then, by Propositions 2.18 and 2.20, $\frac{\sin s|\cdot|}{|\cdot|}$ is strongly X -positive definite for certain subsets X of \mathbb{R}^3 and any $s > 0$. The latter is equivalent to the invertibility of the matrices

$$\mathcal{M}(t) := \left(\delta_{kj} + \frac{\sin(\sqrt{t}|x_k - x_j|)}{\sqrt{t}|x_k - x_j| + \delta_{kj}} \right)_{j,k=1}^{\infty} \quad \text{for} \quad t \in \mathbb{R}_+$$

and plays a crucial role in the proof of Lemma 5.12.

Notation. Throughout the paper \mathfrak{H} and \mathcal{H} are separable complex Hilbert spaces. We denote by $\mathcal{B}(\mathcal{H}, \mathfrak{H})$ the bounded linear operators from \mathcal{H} into \mathfrak{H} , by $\mathcal{B}(\mathcal{H})$ the set $\mathcal{B}(\mathcal{H}, \mathcal{H})$, by $\mathcal{C}(\mathcal{H})$ the closed linear operators on \mathcal{H} and by $\mathfrak{S}_p(\mathcal{H})$ the Neumann-Schatten ideal on \mathcal{H} . In particular, $\mathfrak{S}_{\infty}(\mathcal{H})$ and $\mathfrak{S}_1(\mathcal{H})$ are the ideals of compact operators and trace class operators on \mathcal{H} , respectively.

For closed linear operator T on \mathfrak{H} , we write $\text{dom}(T)$, $\ker(T)$, $\text{ran}(T)$, $\text{gr}(T)$ for the domain, kernel, range, and graph of T , respectively, and $\sigma(T)$ and $\rho(T)$ for the spectrum and the resolvent set of T . The symbols $\sigma_c(T)$, $\sigma_{ac}(T)$, $\sigma_s(T)$, $\sigma_{sc}(T)$, $\sigma_p(T)$ denote the continuous, absolutely continuous, singular, singularly continuous and point spectrum, respectively, of a self-adjoint operator T . Note that $\sigma_s(T) = \sigma_{sc}(T) \cup \sigma_p(T)$ and $\sigma(T) = \sigma_{ac}(T) \cup \sigma_s(T)$. The defect subspaces of a symmetric operator T are denoted by \mathfrak{N}_2 . For basic notions and results on operator theory we refer to [47], [48], [49], and [31].

By $C[0, \infty)$ we mean the Banach space of continuous bounded functions on $[0, \infty)$ and by S_r^n the sphere in \mathbb{R}^n of radius r centered at the origin and $S^n := S_1^n$. Further, $\sum'_{k \in \mathbb{N}}$ denotes the sum over all k such that $k \neq j$ and $\sum_{|k-j|>0}$ is the sum over all $k, j \in \mathbb{N}$ with $k \neq j$.

2 Radial positive definite functions

2.1 Basic definitions

Let $(u, v) = u_1v_1 + \dots + u_nv_n$ be the scalar product of two vectors $u = (u_1, \dots, u_n)$ and $v = (v_1, \dots, v_n)$ from \mathbb{R}^n , $n \in \mathbb{N}$, and let $|u| = |u|_n = \sqrt{(u, u)}$ be the Euclidean norm of u . First we recall some basic facts and notions about positive definite functions [1].

Definition 2.1. [1] A function $g : \mathbb{R}^n \rightarrow \mathbb{C}$ is called *positive definite* if g is continuous at 0 and for arbitrary finite sets $\{x_1, \dots, x_m\}$ and $\{\xi_1, \dots, \xi_m\}$, where $x_k \in \mathbb{R}^n$ and $\xi_k \in \mathbb{C}$, we have

$$\sum_{k,j=1}^m \xi_k \bar{\xi}_j g(x_k - x_j) \geq 0. \quad (2.1)$$

The set of positive definite function on \mathbb{R}^n is denoted by $\Phi(\mathbb{R}^n)$.

Clearly, a function g on \mathbb{R}^n is positive definite if and only if it is continuous at 0 and the matrix $G(X) = (g_{kj} := g(x_k - x_j))_{k,j=1}^m$ is *positive semi-definite* for any finite subset $X = \{x_j\}_1^m$ of \mathbb{R}^n .

The following classical *Bochner theorem* gives a description of the class $\Phi(\mathbb{R}^n)$.

Theorem 2.2. [16] A function $g(\cdot)$ is positive definite on \mathbb{R}^n if and only if there is a finite nonnegative Borel measure μ on \mathbb{R}^n such that

$$g(x) = \int_{\mathbb{R}^n} e^{i(u,x)} d\mu(u) \text{ for all } x \in \mathbb{R}^n. \quad (2.2)$$

Let us continue with a number of further basic definitions.

Definition 2.3. Let g be a positive definite function on \mathbb{R}^n and let X be a subset of \mathbb{R}^n .

(i) We say that g is *strongly X -positive definite* if there exists a constant $c > 0$ such that

$$\sum_{k,j=1}^m \xi_k \bar{\xi}_j g(x_k - x_j) > c \sum_{k=1}^m |\xi_k|^2, \quad \xi = \{\xi_1, \dots, \xi_m\} \in \mathbb{C}^m \setminus \{0\}. \quad (2.3)$$

for any finite set $\{x_j\}_{j=1}^m$ of distinct points $x_j \in X$.

(ii) It is said that g is *strictly X -positive definite* if (2.3) is satisfied with $c = 0$.

Any strongly X -positive definite g is also strictly X -positive definite. For finite sets $X = \{x_j\}_1^m$ both notions are equivalent by the compactness of the sphere in \mathbb{C}^m .

The following problem seems to be important and difficult.

Problem: Let g be a positive definite function on \mathbb{R}^n . Characterize those countable subsets X of \mathbb{R}^n for which g is strictly X -positive definite and strongly X -positive definite, respectively.

We now define three other basic concepts which will be crucial in what follows.

Definition 2.4. [56] Let $F = \{f_k\}_{k=1}^\infty$ be a sequence of vectors of a Hilbert space \mathcal{H} .

(i) This sequence is called a *Riesz-Fischer sequence* if there exists a constant $c > 0$ such that

$$\left\| \sum_{k=1}^m \xi_k f_k \right\|_{\mathcal{H}}^2 \geq c \sum_{k=1}^m |\xi_k|^2 \quad \text{for all } (\xi_1, \dots, \xi_m) \in \mathbb{C}^m \quad \text{and } m \in \mathbb{N}. \quad (2.4)$$

(ii) The sequence F is said to be a *Bessel sequence* if there is a constant $C > 0$ such that

$$\left\| \sum_{k=1}^m \xi_k f_k \right\|_{\mathcal{H}}^2 \leq C \sum_{k=1}^m |\xi_k|^2 \quad \text{for all } (\xi_1, \dots, \xi_m) \in \mathbb{C}^m \quad \text{and } m \in \mathbb{N}. \quad (2.5)$$

(iii) The sequence F is called a *Riesz basis* of the Hilbert space \mathcal{H} if its linear span is dense in \mathcal{H} and F is both a Riesz-Fischer sequence and a Bessel sequence.

Note that the definitions of Riesz-Fischer and Bessel sequences given in [56] are different, but they are equivalent to the preceding definition according to [56, Theorem 4.3].

The following proposition contains some slight reformulations of these notions.

If $\mathcal{A} = (a_{kj})_{k,j \in \mathbb{N}}$ is an infinite matrix of complex entries a_{kj} we shall say that \mathcal{A} defines a bounded operator A on the Hilbert space $l^2(\mathbb{N})$ if

$$\langle Ax, y \rangle = \sum_{k,j=1}^{\infty} a_{kj} x_k \overline{y_j} \quad \text{for } x = \{x_k\}_{k \in \mathbb{N}}, y = \{y_k\}_{k \in \mathbb{N}} \in l^2(\mathbb{N}). \quad (2.6)$$

Clearly, if \mathcal{A} defines a bounded operator A , then A is uniquely determined by equation (2.6).

Proposition 2.5. *Suppose that $X = \{x_k\}_1^{\infty}$ is a sequence of pairwise distinct points of \mathbb{R}^n and g is a positive definite function given by (2.2) with measure μ . Let $F = \{f_k := e^{i(\cdot, x_k)}\}_{k=1}^{\infty}$ denote the sequence of exponential functions in the Hilbert space $L^2(\mathbb{R}^n; \mu)$. Then:*

(i) *F is a Riesz-Fischer sequence in $L^2(\mathbb{R}^n; \mu)$ if and only if g is strongly X -positive definite.*

(ii) *F is a Bessel sequence if and only if the Gram matrix*

$$Gr_F = (\langle f_k, f_j \rangle_{L^2(\mathbb{R}^n; \mu)})_{k,j \in \mathbb{N}} = (g(x_k - x_j))_{k,j \in \mathbb{N}} =: Gr_X(g) \quad (2.7)$$

defines a bounded operator on $l^2(\mathbb{N})$.

Proof. Using equation (2.2) we easily derive

$$\sum_{k,j=1}^m \xi_k \overline{\xi_j} g(x_k - x_j) = \int_{\mathbb{R}^n} \left| \sum_{k=1}^m \xi_k e^{i(u, x_k)} \right|^2 d\mu(u) = \int_{\mathbb{R}^n} \left| \sum_{k=1}^m \xi_k f_k(u) \right|^2 d\mu(u) = \left\| \sum_{k=1}^m \xi_k f_k \right\|_{L^2(\mathbb{R}^n; \mu)}^2 \quad (2.8)$$

for arbitrary $m \in \mathbb{N}$ and $\xi = \{\xi_1, \dots, \xi_m\} \in \mathbb{C}^m$. Both statements are immediate from (2.8). \square

Taking in mind further applications to the spectral theory of self-adjoint realizations of \mathfrak{L}_3 we will be concerned with radial positive definite functions. Let us recall the corresponding concepts.

Definition 2.6. Let $n \in \mathbb{N}$. A function $f \in C([0, +\infty))$ is called a *radial positive definite function* of the class Φ_n if $f(|\cdot|_n)$ is a positive definite function on \mathbb{R}^n , i.e., if $f(|\cdot|_n) \in \Phi(\mathbb{R}^n)$.

It is known that $\Phi_{n+1} \subset \Phi_n$ and $\Phi_n \neq \Phi_{n+1}$ for any $n \in \mathbb{N}$ (see, for instance, [54], [58]).

A characterization of the class Φ_n is given by the following *Schoenberg theorem* [50, 51], see, e.g., [1, Theorem 5.4.2] or [11, 53]. Let σ_n denote the normalized surface measure on the unit sphere S^n .

Theorem 2.7. *A function f on $[0, +\infty)$ belongs to the class Φ_n if and only if there exists a positive finite Borel measure ν on $[0, \infty)$ such that*

$$f(t) = \int_0^{+\infty} \Omega_n(rt) d\nu(r), \quad t \in [0, +\infty), \quad (2.9)$$

where

$$\Omega_n(|x|) = \int_{S^n} e^{i\langle u, x \rangle} d\sigma_n(u), \quad x \in \mathbb{R}^n. \quad (2.10)$$

Moreover, we have

$$\Omega_n(t) = \Gamma\left(\frac{n}{2}\right) \left(\frac{2}{t}\right)^{\frac{n-2}{2}} J_{\frac{n-2}{2}}(t) = \sum_{p=0}^{\infty} \left(-\frac{t^2}{4}\right)^p \frac{\Gamma\left(\frac{n}{2}\right)}{p! \Gamma\left(\frac{n}{2} + p\right)}, \quad t \in [0, +\infty). \quad (2.11)$$

The first three functions Ω_n , $n = 1, 2, 3$, can be computed as

$$\Omega_1(t) = \cos t, \quad \Omega_2(t) = J_0(t), \quad \Omega_3(t) = \frac{\sin t}{t}, \quad (2.12)$$

where J_0 is the Bessel function of first kind and order zero (see e.g., [46], p. 261).

It was proved in [21] using Schoenberg's theorem that for each non-constant function $f \in \Phi_n$, $n \geq 2$, the function $f(|\cdot|)$ is strictly X -positive definite for any finite subset X of \mathbb{R}^n .

2.2 Completely monotone functions and strong X -positive definiteness

Definition 2.8. A function $f \in C[0, \infty) \cap C^\infty(0, +\infty)$ is called completely monotone on $[0, \infty)$ if $(-1)^k f^{(k)}(t) \geq 0$ for all $k \in \mathbb{N} \cup \{0\}$ and $t > 0$. The set of such functions is denoted by $M[0, \infty)$.

By Bernstein's theorem [1], p. 204, a function f on $[0, +\infty)$ belongs to the class $M[0, \infty)$ if and only if there exists a finite positive Borel measure τ on $[0, +\infty)$ such that

$$f(t) = \int_0^\infty e^{-ts} d\tau(s), \quad t \in [0, +\infty). \quad (2.13)$$

The measure τ is then uniquely determined by the function f .

Schoenberg noted in [50, 51] that a function f on $[0, +\infty)$ belongs to $\bigcap_{n \in \mathbb{N}} \Phi_n$ if and only if $f(\sqrt{\cdot}) \in M[0, \infty)$. The following statement is an immediate consequence of Schoenberg's result.

Proposition 2.9. *If $f \in M[0, \infty)$, then $f \in \bigcap_{n \in \mathbb{N}} \Phi_n$.*

Proof. For $s \geq 0$ the function $g_s(t) := e^{-s\sqrt{t}}$ is completely monotone for $t > 0$. Schoenberg's result applies to $g_s(t^2)$ and shows that $g_s(t^2) = e^{-st} \in \bigcap_{n \in \mathbb{N}} \Phi_n$. Therefore the integral representation (2.13) implies that $f(\cdot) \in \bigcap_{n \in \mathbb{N}} \Phi_n$. \square

For any sequence $X = \{x_k\}_{k=1}^\infty$ of points of \mathbb{R}^n we set

$$d_*(X) := \inf_{k \neq j} |x_k - x_j|.$$

The following proposition describes a large class of radial positive-definite functions that are strongly X -positive-definite for any sequence X of points of \mathbb{R}^3 such that $d_*(X) > 0$.

Theorem 2.10. *Let f be a nonconstant function of $M[0, \infty)$ and let τ be the representing measure in equation (2.13). Suppose that $X = \{x_k\}_{k=1}^\infty$ is a sequence of points $x_k \in \mathbb{R}^3$. Then:*

- (i) *If $d_*(X) > 0$, then the function $f(|\cdot|)$ is strongly X -positive definite.*
- (ii) *Suppose that $d_*(X) > 0$ and*

$$\int_0^\infty (s + s^{-3}) d\tau(s) < \infty. \quad (2.14)$$

Then the Gram matrix $Gr_X(f) = (f(|x_k - x_j|))_{k,j \in \mathbb{N}}$ defines a bounded operator with bounded inverse on $l^2(\mathbb{N})$.

(iii) If the Gram matrix $Gr_X(f)$ defines a bounded operator with bounded inverse on $l^2(\mathbb{N})$, then $d_(X) > 0$.*

Theorem 2.10 will be proved in Section 3 below. We restate some results derived in this proof in the following corollary. Let $\tilde{\Phi} = \{\tilde{\varphi}_j\}_{j=1}^\infty$, where

$$\tilde{\varphi}_j(x) := \frac{1}{\sqrt{2\pi}} \int_0^{+\infty} \frac{e^{-s|x-x_j|}}{|x-x_j|} d\tau(s), \quad j \in \mathbb{N}. \quad (2.15)$$

Corollary 2.11. *Suppose $X = \{x_j\}_{j=1}^\infty$ is a sequence of points of \mathbb{R}^3 and τ is a finite positive Borel measure on $[0, +\infty)$. Then:*

- (i) *If $d_*(X) > 0$ and $\tau((0, +\infty)) > 0$, then $\tilde{\Phi}$ forms a Riesz-Fischer sequence in $L^2(\mathbb{R}^3)$.*
- (ii) *If $d_*(X) > 0$ and (2.14) holds, then $\tilde{\Phi}$ is a Bessel sequence in $L^2(\mathbb{R}^3)$.*
- (iii) *If $d_*(X) > 0$ and (2.14) is satisfied, then $\tilde{\Phi}$ forms a Riesz basis in its closed linear span.*
- (iv) *If the sequence $\tilde{\Phi}$ is both a Riesz-Fischer and a Bessel sequence in $L^2(\mathbb{R}^3)$, then $d_*(X) > 0$.*

An immediate consequence of the preceding corollary is

Corollary 2.12. *Let f , X and τ be as in Theorem 2.10 and assume that condition (2.14) holds. Then the sequence $\tilde{\Phi} = \{\tilde{\varphi}_j\}_{j=1}^\infty$ forms a Riesz basis in its closed linear span if and only if $d_*(X) > 0$.*

Remark 2.13. Let f be an absolutely monotone function with integral representation (2.13). Then

$$Gr_X(f) = (f(|x_j - x_k|))_{j,k \in \mathbb{N}} = (\langle \tilde{\varphi}_j, \tilde{\varphi}_k \rangle_{L^2(\mathbb{R}^3)})_{j,k \in \mathbb{N}} = Gr_{\tilde{\Phi}}. \quad (2.16)$$

Proposition 2.14. *Suppose that $f \in \Phi_n$ and let ν be the corresponding representing measure from (2.9). Let $X = \{x_k\}_{k=1}^\infty$ be an arbitrary sequence from \mathbb{R}^n . Then f is strongly X -positive definite if and only if there exists a Borel subset $\mathcal{K} \subset (0, +\infty)$ such that $\nu(\mathcal{K}) > 0$ and the system $\{e^{i(\cdot, x_k)}\}_{k=1}^\infty$ forms a Riesz-Fischer sequence in $L^2(S_r^n; \sigma_n)$ for every $r \in \mathcal{K}$.*

Proof. From (2.9) and (2.10) it follows that for $(\xi_1, \dots, \xi_m) \in \mathbb{C}^m$ and $m \in \mathbb{N}$,

$$\sum_{j,k=1}^m \xi_j \bar{\xi}_k f(|x_j - x_k|) = \int_0^{+\infty} \left(\int_{S^n} \left| \sum_{k=1}^m \xi_k e^{i(u, rx_k)} \right|^2 d\sigma_n(u) \right) d\nu(r). \quad (2.17)$$

Suppose that there exists a set \mathcal{K} as stated above. Then for every $r \in \mathcal{K}$ there is a constant $c(r) > 0$ such that

$$\left\| \sum_{k=1}^m \xi_k e^{i(u, rx_k)} \right\|_{L^2(S^n)}^2 \geq c(r) \sum_{k=1}^m |\xi_k|^2. \quad (2.18)$$

Choosing $c(r)$ measurable and combining this inequality with (2.17) we obtain

$$\sum_{j,k=1}^m \xi_j \bar{\xi}_k f(|x_j - x_k|) = \int_{\mathcal{K}} \left(\left\| \sum_{k=1}^m \xi_k e^{i(u, rx_k)} \right\|_{L^2(S^n)}^2 \right) d\nu(r) \geq c \sum_{k=1}^m |\xi_k|^2, \quad (2.19)$$

where $c := \int_{\mathcal{K}} c(r) d\nu(r)$. Since $\nu(\mathcal{K}) > 0$ and $c(r) > 0$, we have $c > 0$. That is, f is strongly X -positive definite.

The converse follows easily from equation (2.17). \square

Remark 2.15. Of course, the set \mathcal{K} in Proposition 2.14 is not unique in general. If the measure ν has an atom $r_0 \in (0, +\infty)$, i.e., $\nu(\{r_0\}) > 0$, then one can choose $\mathcal{K} = \{r_0\}$. For instance, for the function $f(\cdot) = \Omega_n(r_0 \cdot)$ the representative measure from formula (2.9) is the delta measure δ_{r_0} at r_0 . Therefore, $f(\cdot) = \Omega_n(r_0 \cdot)$ is strongly X -positive definite if and only if the system $\{e^{i(\cdot, x_k)}\}_{k=1}^\infty$ forms a *Riesz-Fischer sequence* in $L^2(S_{r_0}^n; \sigma_n)$.

2.3 Strong X -positive definiteness of functions of the class Φ_n

Let $\Lambda = \{\lambda_k\}_1^\infty$ be a sequence of reals. For $r > 0$ let $n(r)$ denote the largest number of points λ_k that are contained in an interval of length r . Then the *upper density* of Λ is defined by

$$D^*(\Lambda) = \lim_{r \rightarrow +\infty} n(r)r^{-1}.$$

Since $n(r)$ is subadditive, it follows that this limit always exists (see e.g. [12]).

In what follows we need the classical result on Riesz-Fischer sequences of exponents in $L^2(-a, a)$.

Proposition 2.16. *Let $\Lambda = \{\lambda_k\}_1^\infty$ be a real sequence and $a > 0$. Set $E(\Lambda) := \{e^{i\lambda_k x}\}_1^\infty$.*

(i) *If $d_*(\Lambda) > 0$ and $D^*(\Lambda) < a/\pi$, then $E(\Lambda)$ is a Riesz-Fischer sequence in $L^2(-a, a)$.*

(ii) *If $E(\Lambda)$ is a Riesz-Fischer sequence in $L^2(-a, a)$, then $d_*(\Lambda) > 0$ and $D^*(\Lambda) \leq a/\pi$.*

Assertion (i) of Proposition 2.16 is a theorem of A. Beurling [12], while assertion (ii) is a result of H.J. Landau [35], see e.g. [57] and [52]. Proposition 2.16 yields the following statement.

Corollary 2.17. *If $d_*(\Lambda) > 0$ and $D^*(\Lambda) = 0$, then $E(\Lambda)$ is a Riesz-Fischer sequence in $L^2(-a, a)$ for all $a > 0$.*

From this corollary it follows that $E(\Lambda)$ is a Riesz-Fischer sequence in $L^2(-a, a)$ for all $a > 0$ if $\lim_{k \rightarrow \infty} (\lambda_{k+1} - \lambda_k) = +\infty$.

Now we are ready to state the main result of this subsection.

Proposition 2.18. *Let $f \in \Phi_n$, $f \neq \text{const}$, and let $X = \{x_k\}_1^\infty$ be a sequence of points $x_k \in \mathbb{R}^n$, $n \geq 2$, of the form $x_k = (0, x_{k2}, \dots, x_{kn})$. If the sequence $X_n := \{x_{kn}\}_{k=1}^\infty$ of n -th coordinates satisfies the conditions $d_*(X_n) > 0$ and $D^*(X_n) = 0$, then f is strongly X -positive definite.*

Proof. By Schoenberg's theorem 2.7, f admits a representation (2.9). Let $\xi = (\xi_1, \dots, \xi_m) \in \mathbb{C}^m$, $m \in \mathbb{N}$. It follows from (2.9) and (2.10) that

$$\sum_{k,j=1}^m \xi_k \bar{\xi}_j f(|x_k - x_j|) = \int_0^{+\infty} \left(\int_{S^n} \left| \sum_{k=1}^m \xi_k e^{i(u, rx_k)} \right|^2 d\sigma_n(u) \right) d\nu(r). \quad (2.20)$$

Next, we transform the integral over S^n in (2.20). Recall that in terms of spherical coordinates

$$u_1 = \cos \varphi_1, \quad u_{n-1} = \sin \varphi_1 \cdots \sin \varphi_{n-2} \cos \varphi_{n-1}, \quad u_n = \sin \varphi_1 \cdots \sin \varphi_{n-2} \sin \varphi_{n-1}, \\ \varphi_1, \dots, \varphi_{n-2} \in [0, \pi] \quad \text{and} \quad \varphi_{n-1} \in [0, 2\pi],$$

the surface measure σ_n on the unit sphere S^n is given by

$$d\sigma_n(u) \equiv d\sigma_n(u_1, \dots, u_n) = \sin^{n-2} \varphi_1 \sin^{n-3} \varphi_2 \cdots \sin \varphi_{n-2} d\varphi_1 \cdots d\varphi_{n-1}.$$

Set $v = (u_2, \dots, u_n)$ and $B_{n-1} := \{v \in \mathbb{R}^{n-1} : |v| \leq 1\}$. Writing $u \in S^n$ as $u = (u_1, v)$, we derive from the previous formula

$$d\sigma_n(u) = \frac{1}{\sqrt{1-|v|^2}} dv, \quad \text{where} \quad u_1^2 + |v|^2 = 1, \quad v \in B_{n-1}. \quad (2.21)$$

Further, we write $v = (w, t)$, where $w \in \mathbb{R}^{n-2}$ and $t \in \mathbb{R}$, and $x_k = (0, x_{k2}, \dots, x_{kn}) = (0, y_k, x_{kn})$, where $y_k \in \mathbb{R}^{n-2}$. Then we have $(u, rx_k) = r(w, y_k) + rt x_{kn}$. Let B_{n-2} denote the unit ball $B_{n-2} := \{w \in \mathbb{R}^{n-2} : |w| \leq 1\}$ in \mathbb{R}^{n-2} . Using the equality (2.21) we then compute

$$\begin{aligned} \int_{S^n} \left| \sum_{k=1}^m \xi_k e^{i(u, rx_k)} \right|^2 d\sigma_n(u) &= \int_{B_{n-1}} \left| \sum_{k=1}^m \xi_k e^{ir(w, y_k)} e^{irt x_{kn}} \right|^2 \frac{1}{\sqrt{1-|v|^2}} dv \\ &\geq \int_{B_{n-1}} \left| \sum_{k=1}^m \xi_k e^{ir(w, y_k)} e^{irt x_{kn}} \right|^2 dv \\ &= \int_{B_{n-2}} \left(\int_{-\sqrt{1-|w|^2}}^{\sqrt{1-|w|^2}} \left| \sum_{k=1}^m \xi_k e^{ir(w, y_k)} e^{irt x_{kn}} \right|^2 dt \right) dw \\ &= \int_{B_{n-2}} r^{-1} \left(\int_{-r\sqrt{1-|w|^2}}^{r\sqrt{1-|w|^2}} \left| \sum_{k=1}^m (\xi_k e^{ir(w, y_k)}) e^{is x_{kn}} \right|^2 ds \right) dw. \end{aligned} \quad (2.22) \quad (2.23)$$

Since $d_*(X_n) > 0$ and $D^*(X_n) = 0$ by assumption, Corollary 2.17 implies that for any $a > 0$ the sequence $\{e^{is x_{kn}}\}_{k=1}^\infty$ is a Riesz-Fischer sequence in $L^2(-a, a)$. That is, there exists a constant $c(a) > 0$ such that

$$\int_{-a}^a \left| \sum_{k=1}^m (\xi_k e^{ir(w, y_k)}) e^{is x_{kn}} \right|^2 ds \geq c(a) \sum_{k=1}^m |\xi_k e^{ir(w, y_k)}|^2 = c(a) \sum_{k=1}^m |\xi_k|^2.$$

Inserting this inequality, applied with $a = r\sqrt{1-|w|^2} > 0$, into (2.23) and then (2.23) into (2.20) we obtain

$$\begin{aligned} \sum_{k,j=1}^m \xi_k \bar{\xi}_j f(|x_k - x_j|) &\geq \int_0^{+\infty} \left(\int_{B_{n-2}} r^{-1} \left(\int_{-r\sqrt{1-|w|^2}}^{r\sqrt{1-|w|^2}} \left| \sum_{k=1}^m (\xi_k e^{ir(w,y_k)}) e^{isx_{nk}} \right|^2 ds \right) dw \right) d\tilde{\nu}(r) \\ &\geq \int_0^{+\infty} \left(\int_{B_{n-2}} r^{-1} c(r\sqrt{1-|w|^2}) \left(\sum_{k=1}^m |\xi_k|^2 \right) dw \right) d\tilde{\nu}(r) \\ &\geq \left(\int_0^{+\infty} \int_{B_{n-2}} r^{-1} c(r\sqrt{1-|w|^2}) dw d\tilde{\nu}(r) \right) \sum_{k=1}^m |\xi_k|^2. \end{aligned}$$

The double integral in front of the last sum is a finite constant, say γ , by construction. Since f is not constant by assumption, $\tilde{\nu}((0, +\infty)) > 0$. Therefore, since $r^{-1}c(r\sqrt{1-|w|^2}) > 0$ for all $r > 0$ and $|w| < 1$, we conclude that $\gamma > 0$. This shows that f is strongly X -positive definite. \square

Assuming $f \in \Phi_{n+1}$ rather than $f \in \Phi_n$ we obtain the following corollary.

Corollary 2.19. *Assume that $f \in \Phi_{n+1}$ and f is not constant. Let $X = \{x_k\}_1^\infty$ be a sequence of points $x_k = (x_{k1}, x_{k2}, \dots, x_{kn}) \in \mathbb{R}^n$. If the sequence $X_n := \{x_{kn}\}_{k=1}^\infty$ of n -th coordinates satisfies the conditions $d_*(X_n) > 0$ and $D^*(X_n) = 0$, then f is strongly X -positive definite.*

Proof. We identify \mathbb{R}^n with the subspace $\mathbf{0} \oplus \mathbb{R}^n$ of \mathbb{R}^{n+1} . Then X is identified with the sequence $\hat{X} = \{(0, x_k)\}_{k=1}^\infty$. Since $f \in \Phi_{n+1}$, Proposition 2.18 applies to the sequence \hat{X} , so f is strongly \hat{X} -positive definite. Hence it is strongly X -positive definite. \square

The next proposition gives a more precise result for a sequence $X = \{x_k\}_{k=1}^\infty$ of \mathbb{R}^3 which are located on a line.

Proposition 2.20. *Suppose that $\Lambda = \{\lambda_k\}_1^\infty$ is a real sequence and $r > 0$. Let X be the sequence $X = \{x_k := (0, 0, \lambda_k)\}_{k=1}^\infty$ in \mathbb{R}^3 and let $f_r(x) := \Omega_3(r|x|)$, $x \in \mathbb{R}^3$.*

(i) *If $d_*(\Lambda) > 0$ and $D^*(\Lambda) < r/\pi$, then the functions f_r is strongly X -positive definite.*

(ii) *If f_r is strongly X -positive definite, then $d_*(\Lambda) > 0$ and $D^*(\Lambda) \leq r/\pi$.*

Proof. Suppose that $\xi = (\xi_1, \dots, \xi_m) \in \mathbb{C}^m$, $m \in \mathbb{N}$. We introduce spherical coordinates on the unit sphere S^2 in \mathbb{R}^3 by

$$u_1 = \sin \theta \cos \varphi, \quad u_2 = \sin \theta \sin \varphi, \quad u_3 = \cos \theta, \quad \text{where } \theta \in [0, \pi], \varphi \in [0, 2\pi].$$

Then the surface measure σ_2 on the sphere S^2 is given by $d\sigma_2(u) = \sin \theta d\varphi d\theta$ and $(u, rx_k) = r\lambda_k \cos \theta$. Using these facts and equation (2.10) we compute

$$\begin{aligned} \sum_{k,j=1}^m \xi_k \bar{\xi}_j f_r(|x_k - x_j|) &= \sum_{k,j=1}^m \xi_k \bar{\xi}_j \Omega_3(r|x_k - x_j|) = \int_{S^2} \left| \sum_{k=1}^m \xi_k e^{i(u, rx_k)} \right|^2 d\sigma_2(u) \\ &= \int_0^{2\pi} \int_0^\pi \left| \sum_{k=1}^m \xi_k e^{ir\lambda_k \cos \theta} \right|^2 \sin \theta d\varphi d\theta = 2\pi \int_0^\pi \left| \sum_{k=1}^m \xi_k e^{ir\lambda_k \cos \theta} \right|^2 \sin \theta d\theta. \end{aligned}$$

Transforming the latter integral by setting $t = r \cos \theta$ we obtain

$$\sum_{k,j=1}^m \xi_k \bar{\xi}_j f(|x_k - x_j|) = \frac{2\pi}{r} \int_{-r}^r \left| \sum_{k=1}^m \xi_k e^{i\lambda_k t} \right|^2 dt. \quad (2.24)$$

Equality (2.24) is the crucial step for the proof of Proposition 2.20.

(i): Since $d_*(\Lambda) > 0$ and $D^*(\Lambda) < r/\pi$, $E(\Lambda) = \{e^{i\lambda_k t}\}_{k=1}^\infty$ is a Riesz-Fischer sequence in $L^2(-r, r)$ by Proposition 2.16(i). This means that there exists a constant $c > 0$ such that

$$\int_{-r}^r \left| \sum_{k=1}^m \xi_k e^{i\lambda_k t} \right|^2 dt \geq c \sum_{k=1}^m |\xi_k|^2.$$

Combined with (2.24) it follows that f is strongly X -positive definite.

(ii): Since f is strongly X -positive definite, there is a constant $c > 0$ such that

$$\sum_{k,j=1}^m \xi_k \bar{\xi}_j f(|x_k - x_j|) \geq c \sum_{k=1}^m |\xi_k|^2$$

Because of (2.24) this implies that $E(\Lambda)$ is strongly X -positive definite. Therefore, $d_*(\Lambda) > 0$ and $D^*(\Lambda) \leq r/\pi$ by Proposition 2.16(ii). \square

Corollary 2.21. *Assume the conditions of Proposition 2.20 and $r_0 > 0$. Then the functions f_r are strongly X -positive definite for any $r \in (0, r_0)$ if and only if $d_*(\Lambda) > 0$ and $D^*(\Lambda) = 0$.*

2.4 Boundedness of Gram matrices

Here we discuss the question of when the Gram matrix (2.7) defines a bounded operator on $l^2(\mathbb{N})$. A standard criterion for showing that a matrix defines a bounded operator is *Schur's test*. It can be stated as follows:

Lemma 2.22. *Let $\mathcal{A} = (a_{kj})_{k,j \in \mathbb{N}}$ be an infinite hermitian matrix satisfying*

$$C := \sup_{j \in \mathbb{N}} \sum_{k=1}^{\infty} |a_{kj}| < \infty. \quad (2.25)$$

Then the matrix \mathcal{A} defines a bounded self-adjoint operator A on $l^2(\mathbb{N})$ and we have $\|A\| \leq C$.

A proof of Lemma 2.22 can be found, e.g., in [56], p. 159.

Lemma 2.23. *Let $\mathcal{A} = (a_{kj})_{k,j \in \mathbb{N}}$ be an infinite hermitian matrix. Suppose that $\{a_{kj}\}_{k=1}^\infty \in l^2(\mathbb{N})$ for all $j \in \mathbb{N}$ and*

$$\lim_{m \rightarrow \infty} \left(\sup_{j \geq m} \sum_{k \geq m} |a_{kj}| \right) = 0. \quad (2.26)$$

Then the hermitian matrix $\mathcal{A} = (a_{kj})_{k,j \in \mathbb{N}}$ defines a compact self-adjoint operator on $l^2(\mathbb{N})$.

Proof. For $m \in \mathbb{N}$ let \mathcal{A}_m denote the matrix $(a_{kj}^{(m)})_{k,j \in \mathbb{N}}$, where $a_{kj}^{(m)} := 0$ if either $k \geq m$ or $j \geq m$ and $a_{kj}^{(m)} = a_{kj}$ otherwise. Clearly, \mathcal{A}_m defines a bounded operator A_m on $l^2(\mathbb{N})$. From (2.26) it follows that the matrix $\mathcal{A} - \mathcal{A}_m$ satisfies condition (2.25) for large m , so $\mathcal{A} - \mathcal{A}_m$ defines a bounded operator B_m . Therefore \mathcal{A} defines the bounded self-adjoint operator $A := A_m + B_m$.

Let $\varepsilon > 0$ be given. By (2.26), there exists m_0 such that $\sum_{k \geq m} |a_{jk}| < \varepsilon$ for $m > m_0$ and $j > m_0$. Using the latter, the Cauchy-Schwarz inequality and the relation $a_{kj} = a_{jk}$ we derive

$$\begin{aligned} \|B_m x\|^2 &= \sum_{j>m} \left| \sum_{k>m} a_{jk} x_k \right|^2 \leq \sum_{j>m} \left(\sum_{k>m} |a_{jk}| \right) \left(\sum_{k>m} |a_{jk}| |x_k|^2 \right) \\ &\leq \varepsilon \sum_{k>m} \sum_{j>m} |a_{kj}| |x_k|^2 \leq \varepsilon^2 \sum_{k>m} |x_k|^2 \leq \varepsilon^2 \|x\|^2 \end{aligned}$$

for $x = \{x_j\}_1^\infty \in l^2(\mathbb{N})$ and $m > m_0$. This proves that $\lim_m \|B_m\| = \lim_m \|A - A_m\| = 0$. Obviously, A_m is compact, because it has finite rank. Therefore, A is compact. \square

An immediate consequence of Lemma 2.23 is the following corollary.

Corollary 2.24. *If $\mathcal{A} = (a_{kj})_{k,j \in \mathbb{N}}$ is an infinite hermitian matrix satisfying*

$$\lim_{m \rightarrow \infty} \left(\sup_{j \in \mathbb{N}} \sum_{k \geq m} |a_{jk}| \right) = 0, \quad (2.27)$$

then the matrix \mathcal{A} defines a compact self-adjoint operator on $l^2(\mathbb{N})$.

Proposition 2.25. *Let $f \in \Phi_n$, $n \geq 2$, and let ν be the representing measure in equation (2.9). Let $X = \{x_k\}_1^\infty$ be a sequence of pairwise different points $x_k \in \mathbb{R}^n$. Suppose that for each $j, k \in \mathbb{N}$, $j \neq k$, there are positive numbers α_{kj} such that*

$$K := \sup_{j \in \mathbb{N}} \sum'_{k \in \mathbb{N}} \frac{1}{(\alpha_{kj} |x_k - x_j|)^{\frac{n-1}{2}}} < \infty, \quad (2.28)$$

$$L := \sup_{j \in \mathbb{N}} \sum'_{k \in \mathbb{N}} \nu([0, \alpha_{kj}]) < \infty, \quad (2.29)$$

Then the matrix $Gr_X(f) := (f(|x_k - x_j|))_{k,j \in \mathbb{N}}$ defines a bounded self-adjoint operator on $l^2(\mathbb{N})$.

Proof. By (2.11) the function $\Omega_n(t)$ has an alternating power series expansion and $\Omega_n(0) = 1$. Therefore we have $\Omega_n(t) \leq 1$ for $t \in [0, \infty)$. It is well-known (see, e.g., [46], p. 266) that the Bessel function $J_{\frac{n-2}{2}}(t)$ behaves asymptotically as $\sqrt{\frac{2}{\pi t}}$ as $t \rightarrow \infty$. Therefore, it follows from (2.11) that there exists a constant C_n such that

$$|\Omega_n(t)| \leq C_n t^{\frac{1-n}{2}} \quad \text{for } t \in (0, \infty). \quad (2.30)$$

Using these facts and the assumptions (2.28) and (2.29) we obtain

$$\begin{aligned} \sum'_{k \in \mathbb{N}} f(|x_k - x_j|) &= \sum'_{k \in \mathbb{N}} \int_0^\infty \Omega_n(r |x_k - x_j|) d\nu(r) \\ &\leq \sum'_{k \in \mathbb{N}} \left(\int_0^{\alpha_{kj}} 1 d\nu(r) + C_n \int_{\alpha_{kj}}^\infty (r |x_k - x_j|)^{\frac{1-n}{2}} d\nu(r) \right) \\ &\leq \sum'_{k \in \mathbb{N}} \nu([0, \alpha_{kj}]) + \sum'_{k \in \mathbb{N}} C_n \int_{\alpha_{kj}}^\infty (\alpha_{kj} |x_k - x_j|)^{\frac{1-n}{2}} d\nu(r) \\ &= L + C_n \left(\sum'_{k \in \mathbb{N}} (\alpha_{kj} |x_k - x_j|)^{\frac{1-n}{2}} \right) \nu(\mathbb{R}) \leq L + C_n K \nu(\mathbb{R}), \end{aligned}$$

so that

$$\sup_{j \in \mathbb{N}} \sum_{k=1}^{\infty} f(|x_k - x_j|) \leq f(0) + L + C_n K \nu(\mathbb{R}) < \infty. \quad (2.31)$$

This shows that the assumption (2.25) of the Schur test is fulfilled, so the matrix $Gr_X(f)$ defines a bounded operator by Lemma 2.22. \square

The assumptions (2.29) and (2.28) are a growth condition of the measure ν at zero combined with a density condition for the set of points x_k . Let us assume that $\nu([0, \varepsilon]) = 0$ for some $\varepsilon > 0$. Setting $\alpha_{kj} = \varepsilon$ in Proposition 2.25, (2.29) is trivially satisfied and (2.28) holds whenever

$$\sup_{j \in \mathbb{N}} \sum'_{k \in \mathbb{N}} \frac{1}{|x_k - x_j|^{\frac{n-1}{2}}} < \infty. \quad (2.32)$$

Because of its importance we restate this result in the special case when $\nu = \delta_r$ is a delta measure at $r \in (0, \infty)$ separately as

Corollary 2.26. *If $X = \{x_k\}_1^\infty$ is a sequence of pairwise distinct points $x_k \in \mathbb{R}^n$ satisfying (2.32), then for any $r > 0$ the infinite matrix $(\Omega_n(r|x_k - x_j|))_{k,j \in \mathbb{N}}$ defines a bounded operator on $l^2(\mathbb{N})$.*

Applying the Schur test one can derive a number of further results when the matrices $Gr_X(f)$ and $(\Omega_n(r|x_k - x_j|))_{k,j \in \mathbb{N}}$ define bounded operators on $l^2(\mathbb{N})$. An example is the next proposition.

Proposition 2.27. *Suppose $X = \{x_k\}_1^\infty$ is a sequence of distinct points $x_k \in \mathbb{R}^3$ such that*

$$K := \sup_{j \in \mathbb{N}} \sum'_{k \in \mathbb{N}} \frac{1}{|x_k - x_j|} < \infty. \quad (2.33)$$

Let $r \in (0, +\infty)$ and let \mathcal{A} be the infinite matrix given by

$$\Omega_3(t, X) := (\Omega_3(t|x_k - x_j|))_{k,j \in \mathbb{N}} = \left(\frac{\sin(t|x_k - x_j|)}{t|x_k - x_j|} \right)_{k,j \in \mathbb{N}}, \quad (2.34)$$

where we set $\frac{\sin 0}{0} := 1$. If $r^{-1}K < 1$, then \mathcal{A} defines a bounded self-adjoint operator A on $l^2(\mathbb{N})$ with bounded inverse; moreover, $\|A\| \leq 1 + r^{-1}K$ and $\|A^{-1}\| \leq (1 - r^{-1}K)^{-1}$.

Proof. Set $\mathcal{S} \equiv (a_{kj})_{k,j \in \mathbb{N}} := \mathcal{A} - I$, where I is the identity matrix. Since $a_{kk} = 0$, one has

$$\sup_{j \in \mathbb{N}} \sum_k |a_{kj}| = \sup_{j \in \mathbb{N}} \sum'_k \left| \frac{\sin(r|x_k - x_j|)}{r|x_k - x_j|} \right| \leq r^{-1} \sup_{j \in \mathbb{N}} \sum'_k \frac{1}{|x_k - x_j|} = r^{-1}K.$$

This shows that the Hermitean matrix \mathcal{S} satisfies the assumption (2.25) of Lemma 2.22 with $C \leq r^{-1}K$. Thus \mathcal{S} is the matrix of a bounded self-adjoint operator S such that $\|S\| \leq r^{-1}K$. We have $\mathcal{S} := \mathcal{A} - I$. This implies that \mathcal{A} is the matrix of a bounded self-adjoint operator $A = I + S$ and $\|A\| \leq 1 + r^{-1}K$. Since $r^{-1}K < 1$, A has a bounded inverse and $\|A^{-1}\| \leq (1 - r^{-1}K)^{-1}$. \square

3 Riesz bases of defect subspaces and the property of strong X -positive definiteness

Let Δ denote the Laplacian on \mathbb{R}^3 with domain $\text{dom}(-\Delta) = W^{2,2}(\mathbb{R}^3)$ in $L^2(\mathbb{R}^3)$. It is well known that $-\Delta$ is self-adjoint. We fix a sequence $X = \{x_j\}_{j=1}^\infty$ of pairwise distinct points $x_j \in \mathbb{R}^3$ and denote by H the restriction

$$H := -\Delta \upharpoonright \text{dom } H, \quad \text{dom } H = \{f \in W^{2,2}(\mathbb{R}^3) : f(x_j) = 0 \text{ for all } j \in \mathbb{N}\}. \quad (3.1)$$

We abbreviate $r_j := |x - x_j|$ for $x = (x^1, x^2, x^3) \in \mathbb{R}^3$. For $z \in \mathbb{C} \setminus [0, +\infty)$ we denote by \sqrt{z} the branch of the square root of z with positive imaginary part.

Further, let us recall the formula for the resolvent $(-\Delta - zI)^{-1}$ on $L^2(\mathbb{R}^3)$ (see [42]):

$$((-\Delta - zI)^{-1}f)(x) = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{e^{i\sqrt{z}|x-t|}}{|x-t|} f(t) dt, \quad f \in L^2(\mathbb{R}^3). \quad (3.2)$$

Lemma 3.1. *The sequence $E := \{\frac{1}{\sqrt{2\pi}}\varphi_j\}_{j=1}^\infty = \{\frac{1}{\sqrt{2\pi}}\frac{e^{-|x-x_j|}}{|x-x_j|}\}_{j=1}^\infty$ is normed and complete in the defect subspace $\mathfrak{N}_{-1}(\subset L^2(\mathbb{R}^3))$ of the operator H .*

Proof. Suppose that $f \in \mathfrak{N}_{-1}$ and $f \perp E$. Then $u := (I - \Delta)^{-1}f \in W^{2,2}(\mathbb{R}^3)$. By (3.2), we have

$$u(x) = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{e^{-|x-t|}}{|x-t|} f(t) dt. \quad (3.3)$$

Therefore, the orthogonality condition $f \perp E$ means that

$$0 = \langle f, \varphi_j \rangle = \frac{1}{4\pi} \int_{\mathbb{R}^3} f(t) \frac{e^{-|t-x_j|}}{|t-x_j|} dt = u(x_j), \quad j \in \mathbb{N}. \quad (3.4)$$

By (3.4) and (3.1), $u \in \text{dom}(H)$ and $f = (I - \Delta)u = (I + H)u \in \text{ran}(I + H)$. Thus,

$$f \in \mathfrak{N}_{-1} \cap \text{ran}(I + H) = \{0\},$$

i.e. $f = 0$ and the system E is complete.

The function $e^{-|\cdot|}(\in W^{2,2}(\mathbb{R}^3))$ is a (generalized) solution of the equation $(I - \Delta)e^{-|x|} = 2\frac{\exp(-|x|)}{|x|}$. Therefore it follows from (3.3) with $f = f_y(x) := \frac{e^{-|x-y|}}{|x-y|}$ that

$$\frac{e^{-|x-y|}}{2} = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{e^{-|x-t|}}{|x-t|} \cdot \frac{e^{-|t-y|}}{|t-y|} dt. \quad (3.5)$$

Setting here $x = y = x_j$ we get $\|\varphi_j\|^2 = 2\pi$, i.e., the system E is normed. \square

In order to state the next result we need the following definition.

Definition 3.2. A sequence $\{f_j\}_{j=1}^\infty$ of vectors of a Hilbert space is called *w-linearly independent* if for any complex sequence $\{c_j\}_{j=1}^\infty$ the relations

$$\sum_{j=1}^\infty c_j f_j = 0 \quad \text{and} \quad \sum_{j=1}^\infty |c_j|^2 \|f_j\|^2 < \infty \quad (3.6)$$

imply that $c_j = 0$ for all $j \in \mathbb{N}$.

Lemma 3.3. Assume that $X = \{x_j\}_1^\infty$ has no finite accumulation points. Then the sequence $E = \{\frac{1}{\sqrt{2\pi}}\varphi_j\}_{j=1}^\infty = \{\frac{1}{\sqrt{2\pi}} \frac{e^{-|x-x_j|}}{|x-x_j|}\}_{j=1}^\infty$ is ω -linearly independent in $\mathfrak{H} = L^2(\mathbb{R}^3)$.

Proof. Assume that for some complex sequence $\{c_j\}_1^\infty$ conditions (3.6) are satisfied with φ_j in place of f_j . By Lemma 3.1, $\|\varphi_j\| = \sqrt{2\pi}$. Hence the second of conditions (3.6) is equivalent to $\{c_j\} \in l^2$. Furthermore, since each function $\varphi_j(x)$ is harmonic in $\mathbb{R}^3 \setminus \{x_j\}$, this implies that the series $\sum_{j=1}^\infty c_j \varphi_j$ converges uniformly on each compact subset of $\mathbb{R}^3 \setminus X$.

Fix $k \in \mathbb{N}$. Since the points x_j are pairwise distinct and the set X has no finite accumulation points, there exist a compact neighborhood U_k of x_k and such that $x_j \notin U_k$ for all $j \neq k$. Then, by the preceding considerations, the series $\sum_{j \neq k} c_j \varphi_j$ converges uniformly on U_k .

From the first equality of (3.6) it follows that

$$-c_k = \sum'_{j \in \mathbb{N}} c_j e^{-|x-x_j|} |x-x_j|^{-1} |x-x_k|$$

for all $x \in U_k$, $x \neq x_k$. Therefore, passing to the limit as $x \rightarrow x_k$ we obtain $c_k = 0$. \square

Definition 3.4. (i) A sequence $\{f_j\}_1^\infty$ in the Hilbert space \mathfrak{H} is called minimal if for any k

$$\text{dist}\{f_k, \mathfrak{H}^{(k)}\} = \varepsilon_k > 0, \quad \mathfrak{H}^{(k)} := \text{span}\{f_j : j \in \mathbb{N} \setminus \{k\}\}, \quad k \in \mathbb{N}. \quad (3.7)$$

(ii) A sequence $\{f_j\}_1^\infty$ is said to be uniformly minimal if $\inf_{k \in \mathbb{N}} \varepsilon_k > 0$.

(iii) A sequence $\{g_j\}_1^\infty \subset \mathfrak{H}$ is called biorthogonal to $\{f_j\}_1^\infty$ if $\langle f_j, g_k \rangle = \delta_{jk}$ for all $j, k \in \mathbb{N}$.

Let us recall two well-known facts (see e.g. [20]): A biorthogonal sequence to $\{f_j\}_1^\infty$ exists if and only if the sequence $\{f_j\}_1^\infty$ is minimal. If this is true, then the biorthogonal sequence is uniquely determined if and only if the set $\{f_j\}_1^\infty$ is complete in \mathfrak{H} .

Recall that the sequence $\{\varphi_j\}$ is complete in \mathfrak{N}_{-1} according to Lemma 3.1.

Lemma 3.5. Assume that $X = \{x_j\}_1^\infty$ has no finite accumulation points.

(i) The sequence $E := \{\varphi_j\}_1^\infty$ is minimal in \mathfrak{N}_{-1} .

(ii) The corresponding biorthogonal sequence $\{\psi_j\}_1^\infty$ is also complete in \mathfrak{N}_{-1} .

Proof. (i) To prove minimality it suffices to construct a biorthogonal system. Since X has no finite accumulation point, for any $j \in \mathbb{N}$ there exists a function $\tilde{u}_j \in C_0^\infty(\mathbb{R}^3)$ such that

$$\tilde{u}_j(x_j) = 1 \quad \text{and} \quad \tilde{u}_j(x_k) = 0 \quad \text{for} \quad k \neq j. \quad (3.8)$$

Moreover, $\tilde{u}_j(\cdot)$ can be chosen compactly supported in a small neighbourhood of x_j .

Let $\tilde{\psi}_j := (I - \Delta)\tilde{u}_j$, $j \in \mathbb{N}$. In general, $\tilde{\psi}_j \notin \mathfrak{N}_{-1}$. To avoid this drawback we put

$$\psi_j := P_{-1}\tilde{\psi}_j \in \mathfrak{N}_{-1} \quad \text{and} \quad g_j := \tilde{\psi}_j - \psi_j, \quad j \in \mathbb{N}, \quad (3.9)$$

where P_{-1} is the orthogonal projection in \mathfrak{H} onto \mathfrak{N}_{-1} . Then $g_j \in \text{ran}(I + H) = \mathfrak{H} \ominus \mathfrak{N}_{-1}$, $j \in \mathbb{N}$. Setting $v_j = (I - \Delta)^{-1}g_j$, we get $v_j \in \text{dom}(H) \subset \text{dom}(\Delta)$. Therefore, by the Sobolev embedding theorem, $v_j \in C(\mathbb{R}^3)$. Together with the sequence $\{\tilde{u}_j\}_1^\infty$ we consider the sequence of functions

$$u_j := \tilde{u}_j - v_j \in W^{2,2}(\mathbb{R}^3), \quad j \in \mathbb{N}. \quad (3.10)$$

Since $v_j \in \text{dom}(H)$, the functions u_j satisfy relations (3.8) as well. Thus,

$$-\Delta u_j + u_j = \psi_j \in \mathfrak{N}_{-1} \quad \text{and} \quad u_j(x_k) = \delta_{kj} \quad \text{for} \quad j, k \in \mathbb{N}. \quad (3.11)$$

Combining these relations with the resolvent formula (3.2) we get

$$\langle \psi_j, \varphi_k \rangle = \frac{1}{4\pi} \int_{\mathbb{R}^3} \psi_j(x) \frac{e^{-|x-x_j|}}{|x-x_j|} dx = (I - \Delta)^{-1} \psi_j = u_j(x_k) = \delta_{kj}, \quad j, k \in \mathbb{N}. \quad (3.12)$$

These relations mean that the sequence $\{\psi_j\}_1^\infty$ is biorthogonal to the sequence $\{\varphi_j\}_1^\infty$. Hence the latter is minimal.

(ii) Let \mathfrak{H}_1 denote the closed linear span of the set $\{u_j; j \in \mathbb{N}\}$ in $W^{2,2}(\mathbb{R}^3)$.

We prove that $W^{2,2}(\mathbb{R}^3)$ is the closed linear span of its subspaces \mathfrak{H}_1 and $\text{dom}(H)$. Indeed, assume that $g \in W^{2,2}(\mathbb{R}^3)$ and has a compact support $K = \text{supp } g$. Then the intersection $X \cap K$ is finite since X has no accumulation points. Therefore the function

$$g_1 = \sum_{x_j \in K} g(x_j) u_j \quad (3.13)$$

is well defined and $g_1 \in \mathfrak{H}_1$. It follows from (3.11) that $g_0 := g - g_1 \in \text{dom}(H)$ and $g = g_1 + g_0$. It remains to note that $C_0^\infty(\mathbb{R}^3)$ is dense in $W^{2,2}(\mathbb{R}^3)$.

Suppose that $f \in \mathfrak{N}_{-1}$ and $\langle f, \psi_j \rangle = 0$, $j \in \mathbb{N}$. Then, by (3.11),

$$0 = \langle f, \psi_j \rangle = \langle f, (-\Delta + I) u_j \rangle, \quad j \in \mathbb{N}. \quad (3.14)$$

The inclusion $f \in \mathfrak{N}_{-1}$ means that $f \perp (I - \Delta) \text{dom}(H)$. Combining this with (3.14) and using that $W^{2,2}(\mathbb{R}^3)$ is the closure of $\mathfrak{H}_1 + \text{dom}(H)$ as shown above, it follows that $f \perp \text{ran}(I - \Delta) = L^2(\mathbb{R}^3)$. Thus $f = 0$ and the sequence $\{\psi_j\}_1^\infty$ is complete. \square

Lemma 3.6. *If $E = \{\varphi_j\}_1^\infty$ is uniformly minimal, then X has no finite accumulation points.*

Proof. Since $\{\varphi_j\}_1^\infty$ is minimal in \mathfrak{N}_{-1} , there exists the biorthogonal sequence $\{\psi_j\}_1^\infty$ in \mathfrak{N}_{-1} . It was already mentioned that the uniform minimality of $E = \{\varphi_j\}_1^\infty$ is equivalent to $\sup_{j \in \mathbb{N}} \|\varphi_j\| \cdot \|\psi_j\| < \infty$. Therefore, since $\|\varphi_j\| = 2\sqrt{\pi}$, by Lemma 3.1, the sequence $(\psi_j; j \in \mathbb{N})$ is uniformly bounded, i.e. $\sup_j \|\psi_j\| =: C_0 < \infty$. Setting $u_j = (I - \Delta)^{-1} \psi_j \in W_2^2(\mathbb{R}^3)$ we conclude that the sequence $\{u_j\}_1^\infty$ is uniformly bounded in $W^{2,2}(\mathbb{R}^3)$, that is, $\sup_{j \in \mathbb{N}} \|u_j\|_{W^{2,2}} = C_1 < \infty$.

Now assume to the contrary that there is a finite accumulation point y_0 of X . Thus, there exists a subsequence $\{x_{j_m}\}_{m=1}^\infty$ such that $y_0 = \lim_{m \rightarrow \infty} x_{j_m}$. By the Sobolev embedding theorem, the set $\{u_j; j \in \mathbb{N}\}$ is compact in $C(\mathbb{R}^3)$. Thus there exists a subsequence of $\{u_{j_m}\}$ which converges uniformly to $u_0 \in C(\mathbb{R}^3)$. Without loss of generality we assume that the sequence $\{u_{j_m}\}$ itself converges to u_0 , i.e. $\lim_{m \rightarrow \infty} \|u_{j_m} - u_0\|_{C(\mathbb{R}^3)} = 0$. Hence

$$1 = u_{j_m}(x_{j_m}) \xrightarrow{m \rightarrow \infty} u_0(y_0) = 1, \quad 0 = u_{j_m}(x_{j_{m-1}}) \xrightarrow{m \rightarrow \infty} u_0(y_0) = 0,$$

which is the desired contradiction. \square

Lemma 3.7. *Suppose that $d_*(X) = 0$. If the matrix $\mathcal{T}_1 := (\frac{1}{2} e^{-|x_j - x_k|})_{j,k \in \mathbb{N}}$ defines a bounded self-adjoint operator T_1 on $l^2(\mathbb{N})$, then $0 \in \sigma_c(T_1)$, hence T_1 has no bounded inverse.*

Proof. Let $\varepsilon > 0$. Since $d_*(X) = 0$, there exist numbers $n_j \in \mathbb{N}$ such that $r_{jk} := |x_{n_j} - x_{n_k}| < \varepsilon$. Let e_n denote the vector $e_n := \{\delta_{p,n}\}_{p=1}^\infty$ of $l^2(\mathbb{N})$. Then $2 T_1(e_j - e_k) = \{e^{-r_{pj}} - e^{-r_{pk}}\}_{p=1}^\infty \in l^2(\mathbb{N})$.

Since $|r_{pj} - r_{pk}| \leq r_{jk} < \varepsilon$ by the triangle inequality, $e^{-\varepsilon} \leq \exp(r_{pj} - r_{pk}) \leq e^\varepsilon$ and hence

$$|e^{-r_{pj}} - e^{-r_{pk}}| = e^{-r_{pj}} |1 - e^{r_{pj} - r_{pk}}| \leq \varepsilon C e^{-r_{pj}}, \quad j, k, p \in \mathbb{N},$$

where $C > 0$ is a constant. Using the assumption that T_1 is bounded we get

$$4\|T_1(e_j - e_k)\|^2 \leq \varepsilon^2 C^2 \sum_p e^{-2r_{pj}} = 4\varepsilon^2 C^2 \|T_1 e_j\|^2 \leq 4\varepsilon^2 C^2 \|T_1\|^2. \quad (3.15)$$

Since $\varepsilon > 0$ is arbitrary and $\|e_j - e_k\| = \sqrt{2}$ for $j \neq k$, it follows that $0 \in \sigma_c(T_1)$. \square

Theorem 3.8. *The sequence $E = \{\varphi_j\}_1^\infty$ forms a Riesz basis of the Hilbert space \mathfrak{N}_{-1} if and only if $d_*(X) > 0$.*

Proof. Sufficiency. Suppose that $d_*(X) > 0$. By Lemmas 3.1 and 3.5, both sequences $\{\varphi_j\}_1^\infty$ and $\{\psi_j\}_1^\infty$ are complete in \mathfrak{N}_{-1} . Therefore, by [20, Theorem 6.2.1]), the sequence $\{\varphi_j\}$ forms a Riesz basis in \mathfrak{N}_{-1} if and only if

$$\sum_{j=1}^\infty |\langle f, \varphi_j \rangle|^2 < \infty \quad \text{and} \quad \sum_{j=1}^\infty |\langle f, \psi_j \rangle|^2 < \infty \quad \text{for all } f \in \mathfrak{N}_{-1}. \quad (3.16)$$

Let B_j denote the ball in \mathbb{R}^3 centered at x_j with the radius $r = d_*(X)/3$, $j \in \mathbb{N}$. Clearly $B_j \cap B_k = \emptyset$ for $j \neq k$. By the Sobolev embedding theorem, there is a constant $C > 0$ such that

$$|v(x_j)| \leq C \|v\|_{W^{2,2}(B_j)}, \quad v \in W^{2,2}(B_j), \quad j \in \mathbb{N}, \quad (3.17)$$

where C is independent of j and $v \in W^{2,2}(B_j)$.

Let $f \in \mathfrak{N}_{-1}$ and set $u = (I - \Delta)^{-1} f \in W^{2,2}(\mathbb{R}^3)$. Combining (3.17) with the representation (3.2) for u we get

$$\sum_{j=1}^\infty |\langle f, \varphi_j \rangle|^2 = \sum_{j=1}^\infty |u(x_j)|^2 \leq C \sum_{j=1}^\infty \|u\|_{W^{2,2}(B_j)}^2 \leq C \|u\|_{W^{2,2}(\mathbb{R}^3)}^2, \quad f \in \mathfrak{N}_{-1}. \quad (3.18)$$

This proves the first inequality of (3.16).

We now derive the second inequality. Let B_0 be the ball centered at zero with the radius $r = d_*(X)/3$. We choose a function $\tilde{u}_0 \in C_0^\infty(\mathbb{R}^3)$ supported in B_0 and satisfying $\tilde{u}_0(0) = 1$. Put

$$\tilde{u}_j(x) := \tilde{u}_0(x - x_j), \quad j \in \mathbb{N}. \quad (3.19)$$

Clearly, the sequence $\{\tilde{u}_j\}_1^\infty$ satisfies conditions (3.8). Then repeating the reasonings of the proof of Lemma 3.5(i) we find a sequence $\{v_j\}_1^\infty$ of vectors from $\text{dom}(H)$ such that the new sequence $\{u_j := \tilde{u}_j - v_j\}_1^\infty$ satisfies relations (3.11). Hence for any $f \in \mathfrak{N}_{-1}$ we have

$$\langle f, \psi_j \rangle = \langle f, (-\Delta + I)u_j \rangle = \langle f, (-\Delta + I)(\tilde{u}_j - v_j) \rangle = \langle f, (-\Delta + I)\tilde{u}_j \rangle, \quad j \in \mathbb{N}. \quad (3.20)$$

Since $\tilde{u}_j(\cdot)$ is supported in the ball B_j , it follows from (3.19) and relations (3.20) that

$$\begin{aligned} \sum_{j=1}^\infty |\langle f, \psi_j \rangle|^2 &= \sum_{j=1}^\infty |\langle f, (-\Delta + I)\tilde{u}_j \rangle|^2 \leq C \sum_{j=1}^\infty \|f\|_{L^2(B_j)}^2 \|\tilde{u}_j\|_{W^{2,2}(B_j)}^2 \\ &= C \sum_{j=1}^\infty \|f\|_{L^2(B_j)}^2 \|\tilde{u}_0\|_{W^{2,2}(B_0)}^2 = C \|\tilde{u}_0\|_{W^{2,2}(B_0)}^2 \sum_{j=1}^\infty \|f\|_{L^2(B_j)}^2 \leq C \|\tilde{u}_0\|_{W^{2,2}(B_0)}^2 \|f\|_{L^2(\mathbb{R}^3)}^2. \end{aligned}$$

Thus, the second inequality of (3.16) is also proved, hence $\{\varphi_j\}$ forms a Riesz basis.

Necessity. Suppose that $d_*(X) = 0$. By [20, Theorem 6.2.1], a sequence $\Psi = \{\psi_j\}_{j=1}^\infty$ of vectors is a Riesz basis of a Hilbert space \mathfrak{H} if and only if it is complete in \mathfrak{H} and its Gram matrix $Gr_\Psi := (\langle \psi_j, \psi_k \rangle)_{j,k \in \mathbb{N}}$ defines a bounded operator on $l^2(\mathbb{N})$ with bounded inverse.

By (3.5), $E = \{\varphi_j\}_{j=1}^\infty$ has the Gram matrix $Gr_E = (\langle \varphi_j, \varphi_k \rangle)_{j,k \in \mathbb{N}} = (\pi e^{-|x_j - x_k|})_{j,k \in \mathbb{N}} = 2\pi \mathcal{T}_1$. Therefore, by Lemma 3.7, if Gr_E defines a bounded operator, this operator is not boundedly invertible. Hence $E = \{\varphi_j\}_{j=1}^\infty$ is not a Riesz basis by the preceding theorem. \square

Remark 3.9. Note that the proof of uniform minimality of the system E is much simpler. Combining (3.19) with (3.20) we obtain

$$|\langle f, \psi_j \rangle| \leq \|f\|_{L^2} \cdot \|(I - \Delta)\tilde{u}_j\|_{L^2} \leq \|f\|_{L^2} \|\tilde{u}_j\|_{W^{2,2}(\mathbb{R}^3)} = \|f\|_{L^2} \|\tilde{u}_0\|_{W^{2,2}(\mathbb{R}^3)}, \quad j \in \mathbb{N}. \quad (3.21)$$

Since $f \in \mathfrak{N}_{-1}$ is arbitrary, one has $\sup_{j \in \mathbb{N}} \|\psi_j\|_{L^2(\mathbb{R}^3)} \leq \|\tilde{u}_0\|_{W^{2,2}(\mathbb{R}^3)}$, so $\{\psi_j\}_{j \in \mathbb{N}}$ is uniformly minimal.

Next we set

$$\varphi_{j,z}(x) := \frac{e^{i\sqrt{z}|x-x_j|}}{|x-x_j|} \quad \text{and} \quad e_{j,z}(x) := e^{i\sqrt{z}|x-x_j|}, \quad j \in \mathbb{N}. \quad (3.22)$$

Clearly, $\varphi_{j,-1} = \varphi_j$, $j \in \mathbb{N}$.

Corollary 3.10. *Suppose that $d_*(X) > 0$. Then for any $z \in \mathbb{C} \setminus [0, +\infty)$, the sequence $E_z := \{\frac{1}{\sqrt{2\pi}}\varphi_{j,z}\}_{j=1}^\infty$ forms a Riesz basis in the deficiency subspace \mathfrak{N}_z of the operator H . Moreover, for $z = -a^2 < 0$ ($a > 0$) the system $\sqrt{a}E_{-a^2} = \{\frac{\sqrt{a}}{\sqrt{2\pi}}\varphi_{j,-a^2}\}_{j=1}^\infty$ is normed.*

Proof. It is easily seen that

$$\int_{\mathbb{R}^3} \frac{e^{-|x-y|}}{|x-y|} \cdot \frac{e^{i\sqrt{z}|y-x_j|}}{|y-x_j|} dy = \int_{\mathbb{R}^3} \frac{e^{i\sqrt{z}|x-y|}}{|x-y|} \cdot \frac{e^{-|y-x_j|}}{|y-x_j|} dy, \quad j \in \mathbb{N}. \quad (3.23)$$

Using (3.2) we can rewrite this equality as

$$(I - \Delta)^{-1}\varphi_{j,z} = (-\Delta - z)^{-1}\varphi_j, \quad j \in \mathbb{N}, \quad z \in \mathbb{C} \setminus \overline{\mathbb{R}}_+. \quad (3.24)$$

Therefore, we have

$$\varphi_{j,z} = U_z \varphi_j, \quad \text{where} \quad U_z := (I - \Delta)(-\Delta - z)^{-1} = I - (1 + z)(\Delta + z)^{-1}. \quad (3.25)$$

Obviously, U_z is a continuous bijection of \mathfrak{N}_{-1} onto \mathfrak{N}_z . Therefore, since $E = E_{-1} = \{\varphi_j\}_{j \in \mathbb{N}}$ is Riesz basis of \mathfrak{N}_{-1} by Theorem 3.8, $E_z = \{\varphi_{j,z}\}_{j=1}^\infty$ is a Riesz basis of \mathfrak{N}_z .

To prove the second statement we note that for any $a > 0$ the function $e^{-a|\cdot|} (\in W^{2,2}(\mathbb{R}^3))$ is a (generalized) solution of the equation $(a^2 I - \Delta)e^{-a|x|} = 2a \frac{\exp(-a|x|)}{|x|}$. Taking this equality into account we obtain from (3.2) with $z = -a^2$ and $f = f_y(x) := \frac{e^{-a|x-y|}}{|x-y|}$ that

$$\frac{e^{-a|x-y|}}{2a} = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{e^{-a|x-t|}}{|x-t|} \cdot \frac{e^{-a|t-y|}}{|t-y|} dt, \quad a > 0. \quad (3.26)$$

Setting here $x = y = x_j$ we get $\|\varphi_{j,-a^2}\|^2 = 2\pi/a$, i.e., the system $\sqrt{a}E_{-a^2}$ is normed. \square

Now we are ready to prove Theorem 2.10.

Proof of Theorem 2.10.

(i): Suppose that $s \in (0, +\infty)$ and set

$$g_s(x) := s^{-1}e^{-s|x|}, \quad \tilde{\varphi}_{j,s}(x) := \frac{1}{\sqrt{2\pi}}\varphi_{j,-s^2}(x) = \frac{1}{\sqrt{2\pi}} \frac{e^{-s|x-x_j|}}{|x-x_j|}, \quad j \in \mathbb{N}.$$

Equation (3.5) shows that $Gr_X(g_s) = (g_s(x_k - x_j))_{k,j \in \mathbb{N}}$ is the Gram matrix of the sequence $E_{-s^2} := \{\tilde{\varphi}_{j,s}\}_{j=1}^\infty$. Since $d_*(X) > 0$ by assumption, E_{-s^2} forms a Riesz basis by Corollary 3.10. Therefore it follows from [20, Theorem 6.2.1] that for any $s > 0$ the Gram matrix $(\langle \tilde{\varphi}_{j,s}, \tilde{\varphi}_{k,s} \rangle_{L^2(\mathbb{R}^3)})_{j,k \in \mathbb{N}} = Gr_X(g_s)$ defines a bounded operator on $l^2(\mathbb{N})$ with bounded inverse. Hence for any $s > 0$ there exist numbers $C(s) > 0$ and $c(s) > 0$ such that

$$C(s) \sum_{j=1}^m |\xi_j|^2 \geq \sum_{j,k=1}^m \langle \tilde{\varphi}_{j,s}, \tilde{\varphi}_{k,s} \rangle_{L^2(\mathbb{R}^3)} \xi_j \bar{\xi}_k = \sum_{j,k=1}^m s^{-1} e^{-s|x_j - x_k|} \xi_j \bar{\xi}_k \geq c(s) \sum_{j=1}^m |\xi_j|^2 \quad (3.27)$$

for all $(\xi_1, \dots, \xi_m) \in \mathbb{C}^m$ and $m \in \mathbb{N}$. Clearly, the function $c(s)$ on $(0, +\infty)$ can be chosen to be measurable. Since $c(s) > 0$ on \mathbb{R}_+ and $\tau(\mathbb{R}_+) > 0$, we have $c := \int_{(0,+\infty)} s c(s) d\tau(s) > 0$. Combining (2.13) with (3.27) we arrive at the inequality

$$\begin{aligned} \sum_{j,k=1}^m f(|x_j - x_k|) \xi_j \bar{\xi}_k &= \int_0^\infty \left(\sum_{j,k=1}^m e^{-s|x_j - x_k|} \xi_j \bar{\xi}_k \right) d\tau(s) \\ &\geq \int_0^\infty s \left(c(s) \sum_{j=1}^m |\xi_j|^2 \right) d\tau(s) = c \sum_{j=1}^m |\xi_j|^2. \end{aligned} \quad (3.28)$$

This means that the function $f(|\cdot|)$ is strongly X -positive definite.

(ii): By (3.25), $U_{-s^2} = (I - \Delta)(-\Delta + s^2)^{-1}$, hence $\|U_{-s^2}\| = \max(1, s^{-2})$. Moreover, by (3.25), $\tilde{\varphi}_{j,s} = U_{-s^2} \tilde{\varphi}_{j,1}$. Using the preceding facts we derive

$$\begin{aligned} \sum_{j,k=1}^m f(|x_j - x_k|) \xi_j \bar{\xi}_k &= \int_0^\infty \left(\sum_{j,k=1}^m e^{-s|x_j - x_k|} \xi_j \bar{\xi}_k \right) d\tau(s) \\ &= \sum_{j,k=1}^m \int_0^{+\infty} s \langle \tilde{\varphi}_{j,s}, \tilde{\varphi}_{k,s} \rangle \xi_j \bar{\xi}_k d\tau(s) = \int_0^{+\infty} s \left\| \sum_{j=1}^m \xi_j \tilde{\varphi}_{j,s} \right\|^2 d\tau(s) \\ &= \int_0^{+\infty} s \left\| U_{-s^2} \left(\sum_{j=1}^m \xi_j \tilde{\varphi}_{j,1} \right) \right\|^2 d\tau(s) \leq \int_0^{+\infty} s \|U_{-s^2}\|^2 \left\| \sum_{j=1}^m \xi_j \tilde{\varphi}_{j,1} \right\|^2 d\tau(s) \\ &= 2 \int_0^{+\infty} s \|U_{-s^2}\|^2 \sum_{j,k=1}^m \langle \tilde{\varphi}_{j,1}, \tilde{\varphi}_{k,1} \rangle \xi_j \bar{\xi}_k d\tau(s) \\ &\leq \int_0^{+\infty} s(1 + s^{-4}) C(1) \left(\sum_{j=1}^m |\xi_j|^2 \right) d\tau(s) = C \sum_{j=1}^m |\xi_j|^2, \end{aligned} \quad (3.30)$$

where $C := C(1) \int_0^{+\infty} (s + s^{-3}) d\tau(s) < \infty$ by assumption (2.14).

It follows from (3.28) and (3.29) that the matrix $Gr_X(f)$ defines a bounded operator with bounded inverse.

(iii) Suppose that $d_*(X) = 0$. Assume to the contrary that the Gram matrix $Gr_X(f)$ defines a bounded operator, say T , with bounded inverse on $l^2(\mathbb{N})$.

Fix $\varepsilon \in (0, \tau([0, \infty)))$. Since the measure τ is finite, there exists $s_0 > 0$ such that

$$\int_{[s_0, \infty)} d\tau(s) < \varepsilon < \tau([0, \infty)). \quad (3.31)$$

By the assumption $d_*(X) = 0$ we can find points $x_k, x_j \in X$, $k, l \in \mathbb{N}$, such that $r_{jk} = |x_j - x_k| \leq s_0^{-1} \ln(1 + \varepsilon (\tau([0, s_0]))^{-1})$. Fix a number $l \in \mathbb{N}$. First suppose $r_{jl} \leq r_{kl}$. Then

$$0 \leq (1 - e^{-s(r_{kl} - r_{jl})})^2 \leq 1 - e^{-sr_{kl}} \leq \frac{\varepsilon (\tau([0, s_0]))^{-1}}{1 + \varepsilon (\tau([0, s_0]))^{-1}} \leq \varepsilon (\tau([0, s_0]))^{-1}, \quad s \in [0, s_0]. \quad (3.32)$$

Using (3.31) and (3.32) we derive

$$\begin{aligned} \left(\int_0^\infty (e^{-sr_{jl}} - e^{-sr_{kl}}) d\tau(s) \right)^2 &= \left(\int_0^\infty (1 - e^{-s(r_{kl} - r_{jl})}) e^{-sr_{jl}} d\tau(s) \right)^2 \\ &\leq \left(\int_{s_0}^\infty (1 - e^{-s(r_{kl} - r_{jl})})^2 d\tau(s) + \int_0^{s_0} (1 - e^{-s(r_{kl} - r_{jl})})^2 d\tau(s) \right) \left(\int_0^\infty e^{-2sr_{jl}} d\tau(s) \right) \\ &\leq 2\varepsilon \int_0^\infty e^{-2sr_{jl}} d\tau(s). \end{aligned} \quad (3.33)$$

If $r_{jl} > r_{kl}$ then the same reasoning yields

$$\left(\int_0^\infty (e^{-sr_{jl}} - e^{-sr_{kl}}) d\tau(s) \right)^2 \leq 2\varepsilon \int_0^\infty e^{-2sr_{kl}} d\tau(s). \quad (3.34)$$

Summing over l in (3.33) resp. (3.34) we obtain

$$\begin{aligned} \|T(e_j - e_k)\|_{l^2(\mathbb{N})}^2 &= \sum_l |\langle T(e_j - e_k), e_l \rangle|^2 = \sum_l \left(\int_0^\infty (e^{-sr_{jl}} - e^{-sr_{kl}}) d\tau(s) \right)^2 \\ &\leq 2\varepsilon \sum_l \left(\int_0^\infty e^{-2sr_{jl}} d\tau(s) + \int_0^\infty e^{-2sr_{kl}} d\tau(s) \right) = 2\varepsilon (\|Te_j\|^2 + \|Te_k\|^2) \leq 4\varepsilon \|T\|^2. \end{aligned} \quad (3.35)$$

and hence

$$4 = \|e_j - e_k\|^2 \leq \|T^{-1}\|^2 \|T(e_j - e_k)\|^2 \leq 4\varepsilon \|T^{-1}\|^2 \|T\|^2 \quad (3.36)$$

for $j \neq k$. Since $\varepsilon > 0$ is arbitrary, this is a contraction. \square

Now we return to the considerations related to Theorem 3.8 and recall the following

Definition 3.11. A basis $\{f_j\}_1^\infty$ of a Hilbert space \mathfrak{H} is called a *Bari basis* if there exists an orthonormal basis $\{g_j\}_1^\infty$ of \mathfrak{H} such that

$$\sum_{j \in \mathbb{N}} \|f_j - g_j\|^2 < \infty. \quad (3.37)$$

It is known that each Bari basis is a Riesz basis. The converse statement is not true.

Proposition 3.12. *Assume that X has no finite accumulation points. Then the sequence $E := \{\frac{1}{\sqrt{2\pi}}\varphi_j\}_{j=1}^\infty := \{\frac{1}{\sqrt{2\pi}}\frac{e^{-|x-x_j|}}{|x-x_j|}\}_{j=1}^\infty$ forms a Bari basis of \mathfrak{N}_{-1} if and only if*

$$\sum_{j,k \in \mathbb{N}, j \neq k} e^{-2|x_j-x_k|} < \infty. \quad (3.38)$$

Moreover, this condition is equivalent to

$$D_\infty := \lim_{n \rightarrow \infty} D(\varphi_1, \dots, \varphi_n) > 0, \quad (3.39)$$

where $D(\varphi_1, \dots, \varphi_n)$ denotes the determinant of the matrix $(\langle \varphi_j, \varphi_k \rangle)_{j,k=1}^n$.

Proof. By (3.5), we have $\langle \varphi_j, \varphi_k \rangle = 2\pi \exp(-|x_j - x_k|)$ for $j, k \in \mathbb{N}$. By Lemma 3.3, the system E is ω -linearly independent. Therefore, by [20, Theorem 6.3.3], E is a Bari basis if and only if

$$(\langle \varphi_j, \varphi_k \rangle - 2\pi \delta_{jk})_{j,k=1}^\infty = 2\pi (\exp(-|x_j - x_k|) - \delta_{jk})_{j,k=1}^\infty \in \mathfrak{S}_2(l^2),$$

i.e. condition (3.38) is satisfied. The second statement follows from [20, Theorem 6.3.1.] \square

4 Operator-Theoretic Preliminaries

4.1 Boundary triplets and self-adjoint relations

Here we briefly recall basic notions and facts on boundary triplets (see [17, 22, 49] for details). In what follows A denotes a densely defined closed symmetric operator on a Hilbert space \mathfrak{H} , $\mathfrak{N}_z := \mathfrak{N}_z(A) = \ker(A^* - z)$, $z \in \mathbb{C}_\pm$, is the defect subspace. We also assume that A has equal deficiency indices $n_+(A) := \dim(\mathfrak{N}_i) = \dim(\mathfrak{N}_{-i}) =: n_-(A)$.

Definition 4.1. [22] A boundary triplet for the adjoint operator A^* is a triplet $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ of an auxiliary Hilbert space \mathcal{H} and of linear mappings $\Gamma_0, \Gamma_1 : \text{dom}(A^*) \rightarrow \mathcal{H}$ such that

(i) the following abstract Green identity holds:

$$(A^*f, g)_{\mathfrak{H}} - (f, A^*g)_{\mathfrak{H}} = (\Gamma_1 f, \Gamma_0 g)_{\mathcal{H}} - (\Gamma_0 f, \Gamma_1 g)_{\mathcal{H}}, \quad f, g \in \text{dom}(A^*). \quad (4.1)$$

(ii) the mapping $(\Gamma_0, \Gamma_1) : \text{dom}(A^*) \rightarrow \mathcal{H} \oplus \mathcal{H}$ is surjective.

With a boundary triplet Π one associates two self-adjoint extensions of A defined by

$$A_0 := A^* \upharpoonright \ker(\Gamma_0) \quad \text{and} \quad A_1 := A^* \upharpoonright \ker(\Gamma_1). \quad (4.2)$$

Definition 4.2. (i) A closed extension \tilde{A} of A is called *proper* if $A \subset \tilde{A} \subset A^*$. The set of all proper extensions of A is denoted by Ext_A .

(ii) Two proper extensions \tilde{A}_1 and \tilde{A}_2 of A are called *disjoint* if $\text{dom}(\tilde{A}_1) \cap \text{dom}(\tilde{A}_2) = \text{dom}(A)$ and *transversal* if, in addition, $\text{dom}(\tilde{A}_1) \dot{+} \text{dom}(\tilde{A}_2) = \text{dom}(A^*)$.

Remark 4.3. (i) If the symmetric operator A has equal deficiency indices $n_+(A) = n_-(A)$, then a boundary triplet $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ for A^* always exists and we have $\dim \mathcal{H} = n_\pm(A)$ [22].

(ii) For each self-adjoint extension \tilde{A} of A there exists a boundary triplet $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ such that $\tilde{A} = A^* \upharpoonright \ker(\Gamma_0) = A_0$.

(iii) If $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ is a boundary triplet for A^* and $B = B^* \in \mathcal{B}(\mathcal{H})$, then the triplet $\Pi_B = \{\mathcal{H}, \Gamma_0^B, \Gamma_1^B\}$ with $\Gamma_1^B := \Gamma_0$ and $\Gamma_0^B := B\Gamma_0 - \Gamma_1$ is also a boundary triplet for A^* .

Boundary triplets for A^* allow one to parameterize the set Ext_A in terms of closed linear relations. For this we recall the following definitions.

Definition 4.4. (i) A linear relation Θ in \mathcal{H} is a linear subspace of $\mathcal{H} \oplus \mathcal{H}$. It is called closed if the corresponding subspace is closed in $\mathcal{H} \oplus \mathcal{H}$.

(ii) A linear relation Θ is called symmetric if $(g_1, f_2) - (f_1, g_2) = 0$ for all $\{f_1, g_1\}, \{f_2, g_2\} \in \Theta$.

(iii) The adjoint relation Θ^* of a linear relation Θ in \mathcal{H} is defined by

$$\Theta^* = \{ \{k, k'\} : (h', k) = (h, k') \text{ for all } \{h, h'\} \in \Theta \}.$$

(iv) A closed linear relation Θ is called self-adjoint if $\Theta = \Theta^*$.

(v) The inverse of a relation Θ is the relation Θ^{-1} defined by $\Theta^{-1} = \{ \{h', h\} : \{h, h'\} \in \Theta \}$.

Definition 4.5. Let Θ be a closed relation in \mathcal{H} . The resolvent set $\rho(\Theta)$ is the set of complex numbers λ such that the relation $(\Theta - \lambda I)^{-1} := \{ \{h' - \lambda h, h\} : \{h, h'\} \in \Theta \}$ is the graph of a bounded operator of $\mathcal{B}(\mathcal{H})$. The complement set $\sigma(\Theta) := \mathbb{C} \setminus \rho(\Theta)$ is called the spectrum of Θ .

For a relation Θ in \mathcal{H} we define the domain $\text{dom}(\Theta)$ and the multi-valued part $\text{mul}(\Theta)$ by

$$\text{dom}(\Theta) = \{h \in \mathcal{H} : \{h, h'\} \in \Theta \text{ for some } h' \in \mathcal{H}\}, \quad \text{mul}(\Theta) = \{h' \in \mathcal{H} : \{0, h'\} \in \Theta\}.$$

Each closed relation Θ is the orthogonal sum of $\Theta_\infty := \{ \{0, f'\} \in \Theta \}$ and $\Theta_{\text{op}} := \Theta \ominus \Theta_\infty$. Then Θ_{op} is the graph of a closed operator, called the operator part of Θ and denoted also by Θ_{op} , and Θ_∞ is a “pure” relation, that is, $\text{mul}(\Theta_\infty) = \text{mul}(\Theta)$.

Suppose that Θ is a self-adjoint relation in \mathcal{H} . Then $\text{mul}(\Theta)$ is the orthogonal complement of $\text{dom}(\Theta)$ in \mathcal{H} and Θ_{op} is a self-adjoint operator in the Hilbert space $\mathcal{H}_{\text{op}} := \overline{\text{dom}(\Theta)}$. That is, Θ is the orthogonal sum of an “ordinary” self-adjoint operator Θ_{op} in \mathcal{H}_{op} and a “pure” relation Θ_∞ in $\mathcal{H}_\infty := \text{mul}(\Theta)$.

Proposition 4.6 ([17, 22, 49]). Let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* . Then the mapping

$$\text{Ext}_A \ni \tilde{A} := A_\Theta \rightarrow \Theta := \Gamma(\text{dom}(\tilde{A})) = \{ \{\Gamma_0 f, \Gamma_1 f\} : f \in \text{dom}(\tilde{A}) \} \quad (4.3)$$

is a bijection of the set Ext_A of all proper extensions of A and the set of all closed linear relations $\tilde{\mathcal{C}}(\mathcal{H})$ in \mathcal{H} . Moreover, the following equivalences hold:

(i) $(A_\Theta)^* = A_{\Theta^*}$ for any linear relation Θ in \mathcal{H} .

(ii) A_Θ is symmetric if and only if Θ is symmetric. Moreover, $n_\pm(A_\Theta) = n_\pm(\Theta)$. In particular, A_Θ is self-adjoint if and only if Θ is self-adjoint.

(iii) The closed extensions A_Θ and A_0 are disjoint if and only if $\Theta = B$ is a closed operator. In this case

$$A_\Theta = A_B = A^* \upharpoonright \text{dom}(A_B), \quad \text{dom}(A_B) = \ker(\Gamma_1 - B\Gamma_0). \quad (4.4)$$

4.2 Weyl function, γ -field and spectra of proper extensions

The notion of the Weyl function and the γ -field of a boundary triplet was introduced in [17].

Definition 4.7 ([17, 49]). Let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* . The operator-valued functions $\gamma(\cdot) : \rho(A_0) \rightarrow \mathcal{B}(\mathcal{H}, \mathfrak{H})$ and $M(\cdot) : \rho(A_0) \rightarrow \mathcal{B}(\mathcal{H})$ defined by

$$\gamma(z) := (\Gamma_0 \upharpoonright \mathfrak{N}_z)^{-1} \quad \text{and} \quad M(z) := \Gamma_1 \gamma(z), \quad z \in \rho(A_0), \quad (4.5)$$

are called the γ -field and the Weyl function, respectively, of $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$.

Note that the γ -field $\gamma(\cdot)$ and the Weyl function $M(\cdot)$ are holomorphic on $\rho(A_0)$.

Recall that a symmetric operator A in \mathfrak{H} is said to be *simple* if there is no non-trivial subspace which reduces it to a self-adjoint operator. In other words, A is simple if it does not admit an (orthogonal) decomposition $A = A' \oplus S$ where A' is a symmetric operator and S is a selfadjoint operator acting on a nontrivial Hilbert space.

It is easily seen (and well-known) that A is simple if and only if $\text{span}\{\mathfrak{N}_z(A) : z \in \mathbb{C} \setminus \mathbb{R}\} = \mathfrak{H}$.

If A is simple, then the Weyl function $M(\cdot)$ determines the boundary triplet Π uniquely up to the unitary equivalence (see [17]). In particular, $M(\cdot)$ contains the full information about the spectral properties of A_0 . Moreover, the spectrum of a proper (not necessarily self-adjoint) extension $A_\Theta \in \text{Ext}_A$ can be described by means of $M(\cdot)$ and the boundary relation Θ .

Proposition 4.8 ([17],[49]). *Let A be a simple densely defined symmetric operator in \mathfrak{H} , $\Theta \in \tilde{\mathcal{C}}(\mathcal{H})$, and $z \in \rho(A_0)$. Then:*

- (i) $z \in \rho(A_\Theta)$ if and only if $0 \in \rho(\Theta - M(z))$;
- (ii) $z \in \sigma_\tau(A_\Theta)$ if and only if $0 \in \sigma_\tau(\Theta - M(z))$, $\tau \in \{p, c\}$.
- (iii) $f \in \ker(A_\Theta - z)$ if and only if $\Gamma_0 f \in \ker(\Theta - M(z))$ and

$$\dim \ker(A_\Theta - z) = \dim \ker(\Theta - M(z)).$$

For any boundary triplet $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ for A^* and any proper extension $A_\Theta \in \text{Ext}_A$ with non-empty resolvent set the following Krein-type resolvent formula holds (cf. [17, 49])

$$(A_\Theta - z)^{-1} = (A_0 - z)^{-1} + \gamma(z)(\Theta - M(z))^{-1}\gamma(\bar{z})^*, \quad z \in \rho(A_\Theta) \cap \rho(A_0). \quad (4.6)$$

It should be emphasized that formulas (4.2) (4.3), and (4.5) express all data occuring in (4.6) in terms of the boundary triplet. These expressions allow one to apply formula (4.6) to boundary value problems.

The following result is deduced from (4.6).

Proposition 4.9 ([17, Theorem 2]). *Let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* and let $\Theta', \Theta \in \tilde{\mathcal{C}}(\mathcal{H})$. Suppose that $\rho(A_{\Theta'}) \cap \rho(A_\Theta) \neq \emptyset$ and $\rho(\Theta') \cap \rho(\Theta) \neq \emptyset$.*

- (i) *For $z \in \rho(A_{\Theta'}) \cap \rho(A_\Theta)$, $\zeta \in \rho(\Theta') \cap \rho(\Theta)$, and $p \in [0, \infty]$ the following equivalence is valid:*

$$(A_{\Theta'} - z)^{-1} - (A_\Theta - z)^{-1} \in \mathfrak{S}_p(\mathfrak{H}) \iff (\Theta' - \zeta)^{-1} - (\Theta - \zeta)^{-1} \in \mathfrak{S}_p(\mathcal{H}). \quad (4.7)$$

In particular, $(A_\Theta - z)^{-1} - (A_0 - z)^{-1} \in \mathfrak{S}_p(\mathfrak{H})$ if and only if $(\Theta - \zeta)^{-1} \in \mathfrak{S}_p(\mathcal{H})$ for $\zeta \in \rho(\Theta)$.

- (ii) *If $\text{dom}(\Theta') = \text{dom}(\Theta)$, then the following implication holds*

$$\overline{\Theta' - \Theta} \in \mathfrak{S}_p(\mathcal{H}) \implies (A_{\Theta'} - z)^{-1} - (A_\Theta - z)^{-1} \in \mathfrak{S}_p(\mathfrak{H}), \quad z \in \rho(A_{\Theta'}) \cap \rho(A_\Theta) \quad (4.8)$$

In particular, if $\Theta', \Theta \in \mathcal{B}(\mathcal{H})$, then (4.7) is equivalent to $\Theta' - \Theta \in \mathfrak{S}_p(\mathcal{H})$.

4.3 Extensions of nonnegative symmetric operators

In this subsection we assume that the symmetric operator A on \mathfrak{H} is *nonnegative*. Then the set $\text{Ext}_A(0, \infty)$ of all nonnegative self-adjoint extensions of A on \mathfrak{H} is not empty. Moreover, there exists a maximal nonnegative extension A_F , called the *Friedrichs' extension*, and a minimal nonnegative extension A_K , called the *Krein's extension*, in the set $\text{Ext}_A(0, \infty)$ and

$$(A_F + x)^{-1} \leq (\tilde{A} + x)^{-1} \leq (A_K + x)^{-1}, \quad x \in (0, \infty), \quad \tilde{A} \in \text{Ext}_A(0, \infty).$$

(For details we refer the reader to [2, Chapter 8], [31, Section 6.2.3] or [49, Sections 13.3, 14.8].)

Proposition 4.10 ([17]). *Let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* such that $A_0 \geq 0$ and let $M(\cdot)$ be the corresponding Weyl function.*

(i) *There exists a lower semibounded self-adjoint linear relation $M(0)$ in \mathcal{H} which is the strong resolvent limit of $M(x)$ as $x \uparrow 0$. Moreover, $M(0)$ is associated with the closed quadratic form*

$$\mathfrak{t}_0[h] := \lim_{x \uparrow 0} (M(x)h, h), \quad \text{dom}(\mathfrak{t}_0) = \{h : \lim_{x \uparrow 0} (M(x)h, h) < \infty\} = \text{dom}((M(0) - M(-a))^{1/2}).$$

(ii) *The Krein extension A_K is given by*

$$A_K = A^* \upharpoonright \text{dom}(A_K), \quad \text{dom}(A_K) = \{f \in \text{dom}(A^*) : \{\Gamma_0 f, \Gamma_1 f\} \in M(0)\}. \quad (4.9)$$

The extensions A_K and A_0 are disjoint if and only if $M(0) \in \mathcal{C}(\mathcal{H})$. In this case $\text{dom}(A_K) = \ker(\Gamma_1 - M(0)\Gamma_0)$.

(iii) *$A_0 = A_F$ if and only if $\lim_{x \downarrow -\infty} (M(x)f, f) = -\infty$ for $f \in \mathcal{H} \setminus \{0\}$.*

(iv) *$A_0 = A_K$ if and only if $\lim_{x \uparrow 0} (M(x)f, f) = +\infty$ for $f \in \mathcal{H} \setminus \{0\}$.*

If A_Θ is lower semibounded, then Θ is lower semibounded too. The converse is not true in general. In order to state the corresponding result we introduce the following definition.

We shall say that $M(\cdot)$ tends uniformly to $-\infty$ as $x \rightarrow -\infty$ if for any $a > 0$ there exists $x_a < 0$ such that $M(x_a) < -a \cdot I_{\mathcal{H}}$. In this case we write $M(x) \rightrightarrows -\infty$ as $x \rightarrow -\infty$.

Proposition 4.11 ([17]). *Suppose that A is a non-negative symmetric operator on \mathfrak{H} and $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ is a boundary triplet for A^* such that $A_0 = A_F$. Let M be the corresponding Weyl function. Then the two assertions*

(i) *a linear relation $\Theta \in \tilde{\mathcal{C}}_{\text{self}}(\mathcal{H})$ is semibounded below,*

(ii) *a self-adjoint extension A_Θ is semibounded below,*

are equivalent if and only if $M(x) \rightrightarrows -\infty$ for $x \rightarrow -\infty$.

Recall that the order relation for lower semibounded self-adjoint operators T_1, T_2 is defined by

$$T_1 \geq T_2 \quad \text{if} \quad \text{dom}(\mathfrak{t}_{T_1}) \subset \text{dom}(\mathfrak{t}_{T_2}) \quad \text{and} \quad \mathfrak{t}_{T_1}[u] \geq \mathfrak{t}_{T_2}[u], \quad u \in \text{dom}(\mathfrak{t}_{T_1}), \quad (4.10)$$

where \mathfrak{t}_{T_j} is the quadratic form associated with T_j .

If T is a self-adjoint operator with spectral measure E_T , put $\kappa_-(T) := \dim \text{ran}(E_T(-\infty, 0))$. For a self-adjoint relation Θ we set $\kappa_-(\Theta) := \kappa_-(\Theta_{op})$, where Θ_{op} is the operator part of Θ . For a quadratic form \mathfrak{t} we denote by $\kappa_-(\mathfrak{t})$ the number of negative squares of \mathfrak{t} (cf. [38]).

Proposition 4.12 ([17]). *Suppose A is a densely defined nonnegative symmetric operator on \mathfrak{H} and $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ is a boundary triplet for A^* such that $A_0 = A_F$. Let M be the Weyl function of this boundary triplet and let Θ be a self-adjoint relation on \mathcal{H} . Then:*

(i) *The self-adjoint extension A_Θ is nonnegative if and only if $\Theta \geq M(0)$.*

(ii) *If A_Θ is lower semibounded and $\text{dom}(\mathfrak{t}_\Theta) \subset \text{dom}(\mathfrak{t}_{M(0)})$, then $\kappa_-(A_\Theta) = \kappa_-(\mathfrak{t}_\Theta - \mathfrak{t}_{M(0)})$. If, in addition, $M(0) \in \mathcal{B}(\mathcal{H})$, then $\kappa_-(A_\Theta) = \kappa_-(\Theta - M(0))$.*

4.4 Absolutely continuous spectrum and the Weyl function

In what follows we will denote

$$M_h(z) := (M(z)h, h), \quad z \in \mathbb{C}_+, \quad \text{and} \quad M_h(x + i0) := \lim_{y \downarrow 0} M_h(x + iy), \quad h \in \mathcal{H}.$$

Since $\text{Im}(M_h(z)) > 0$, $z \in \mathbb{C}_+$, the limit $M_h(x + i0)$ exists and is finite for a.e. $x \in \mathbb{R}$. We put

$$\Omega_{ac}(M_h) := \{x \in \mathbb{R} : 0 < \text{Im } M_h(x) < +\infty\}.$$

We also set $d_M(x) := \text{rank}(\text{Im}(M(x + i0))) \leq \infty$ provided that the weak limit $M(x + i0) := w - \lim_{y \downarrow 0} M(x + iy)$ exists.

Proposition 4.13 ([13]). *Let A be a simple densely defined closed symmetric operator on a separable Hilbert space \mathfrak{H} and let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* with Weyl function M . Assume that $\{h_k\}_{k=1}^N$, $1 \leq N \leq \infty$, is a total set in \mathcal{H} . Recall that A_0 is the self-adjoint operator defined by $A_0 = A^* \upharpoonright \ker(\Gamma_0)$.*

(i) *A_0 has no point spectrum in the interval (a, b) if and only if $\lim_{y \downarrow 0} y M_{h_k}(x + iy) = 0$ for all $x \in (a, b)$ and $k \in \{1, 2, \dots, N\}$.*

(ii) *A_0 has no singular continuous spectrum in the interval (a, b) if the set $(a, b) \setminus \Omega_{ac}(M_{h_k})$ is countable for each $k \in \{1, 2, \dots, N\}$.*

To state the next proposition we need the concept of the ac -closure $\text{cl}_{ac}(\delta)$ of a Borel subset $\delta \subset \mathbb{R}$ introduced independently in [13] and [19]. We refer to [19, 41] for the definition of this notion as well as for its basic properties.

Proposition 4.14 ([40, 41]). *Retain the assumptions of Proposition 4.13. Let B be a self-adjoint operator on \mathcal{H} , $A_B = A^* \upharpoonright \ker(\Gamma_1 - B\Gamma_0)$, and $M_B(z) := (B - M(z))^{-1}$.*

(i) *If the limit $M(x + i0) := w - \lim_{y \downarrow 0} M(x + iy)$ exists a.e. on \mathbb{R} , then $\sigma_{ac}(A_0) = \text{cl}_{ac}(\text{supp}(d_M(x)))$.*

(ii) *For any Borel subset $\mathcal{D} \subset \mathbb{R}$ the ac -parts $A_0 E_{A_0}^{ac}(\mathcal{D})$ and $A_B E_{A_B}^{ac}(\mathcal{D})$ of the operators $A_0 E_{A_0}(\mathcal{D})$ and $A_B E_{A_B}(\mathcal{D})$ are unitarily equivalent if and only if $d_M(x) = d_{M_B}(x)$ a.e. on \mathcal{D} .*

5 Three-dimensional Schrödinger operator with point interactions

First we collect some notation and assumptions that will be kept in this section. Throughout the section we fix a sequence $X = \{x_k\}_{k=1}^\infty$ of points $x_k \in \mathbb{R}^3$ satisfying

$$d_*(X) = \inf_{k, j \in \mathbb{N}, k \neq j} |x_k - x_j| > 0,$$

denote by H the restriction of $-\Delta$ given by (3.1), and set

$$\varphi_{j,z}(x) = \frac{e^{i\sqrt{z}|x-x_j|}}{|x-x_j|} \quad \text{and} \quad e_{j,z}(x) = e^{i\sqrt{z}|x-x_j|}, \quad z \in \mathbb{C} \setminus [0, +\infty), \quad j \in \mathbb{N}. \quad (5.1)$$

Clearly, $\varphi_j = \varphi_{j,-1}$ and $e_j = e_{j,-1}$. Recall from Lemma 3.7 that T_1 is the bounded operator on $l^2(\mathbb{N})$ defined by the matrix $\mathcal{T}_1 := (2^{-1}e^{-|x_j-x_k|})_{j,k \in \mathbb{N}}$.

5.1 Boundary triplets and Weyl functions

The following lemma is a special case of Example 14.3 in [49].

Lemma 5.1. *Let A be a densely defined closed symmetric operator on \mathfrak{H} . Suppose that \tilde{A} is a self-adjoint extension of A on \mathfrak{H} and $-1 \in \rho(\tilde{A})$. Then:*

$$(i) \quad \begin{aligned} \operatorname{dom}(A^*) &= \operatorname{dom} A \dot{+} \ker(A^* + I) \dot{+} (\tilde{A} + I)^{-1} \mathfrak{N}_{-1}, \\ A^*(f_A + f_0 + (\tilde{A} + I)^{-1} f_1) &= Af_A - f_0 + \tilde{A}(\tilde{A} + I)^{-1} f_1, \end{aligned}$$

where $f_A \in \operatorname{dom}(A)$ and $f_0, f_1 \in \mathfrak{N}_{-1} := \ker(A^* + I)$.

(ii) Define $\mathcal{H}' = \mathfrak{N}_{-1}$ and $\Gamma'_j(f_A + f_0 + (\tilde{A} + I)^{-1} f_1) = f_j$ for $j = 0, 1$. Then $\Pi' = \{\mathcal{H}', \Gamma'_0, \Gamma'_1\}$ forms a boundary triplet for A^* .

Proof. Assertion (i) is well known in extension theory (see e.g. [49, formula (14.17)]), so we prove only assertion (ii). Let $f = f_A + f_0 + (I + \tilde{A})^{-1} f_1$ and $g = g_A + g_0 + (I + \tilde{A})^{-1} g_1$, where $f_0, f_1, g_0, g_1 \in \mathfrak{N}_{-1}$. Then

$$\begin{aligned} \langle A^* f, g \rangle - \langle f, A^* g \rangle &= \langle \tilde{A}(I + \tilde{A})^{-1} f_1, g_0 \rangle - \langle f_0, (I + \tilde{A})^{-1} g_1 \rangle \\ &\quad + \langle \tilde{A}(I + \tilde{A})^{-1} f_1, (I + \tilde{A})^{-1} g_1 \rangle - \langle f_0, \tilde{A}(I + \tilde{A})^{-1} g_1 \rangle \\ &\quad + \langle (I + \tilde{A})^{-1} f_1, g_0 \rangle - \langle (I + \tilde{A})^{-1} f_1, \tilde{A}(I + \tilde{A})^{-1} g_1 \rangle \\ &= - \langle f_0, (I + \tilde{A})(I + \tilde{A})^{-1} g_1 \rangle + \langle (I + \tilde{A})(I + \tilde{A})^{-1} f_1, g_0 \rangle \\ &= - \langle f_0, g_1 \rangle_{\mathcal{H}'} + \langle f_1, g_0 \rangle_{\mathcal{H}'} = \langle \Gamma'_1 f, \Gamma'_0 g \rangle_{\mathcal{H}'} - \langle \Gamma'_0 f, \Gamma'_1 g \rangle_{\mathcal{H}'}. \end{aligned} \quad (5.2)$$

The surjectivity of the mapping (Γ'_0, Γ'_1) is obvious. \square

Next we apply Lemma 5.1 to the minimal Schrödinger operator $A = H$.

Proposition 5.2. *Suppose H is the minimal Schrödinger operator defined by (3.1) and $d_*(X) > 0$. Let T_1 be the bounded operator on $l^2(\mathbb{N})$ defined by the matrix $\mathcal{T}_1 := (2^{-1}e^{-|x_j - x_k|})_{j,k \in \mathbb{N}}$. Then*

(i) H is a closed symmetric operator with deficiency indices (∞, ∞) . The defect subspace $\mathfrak{N}_{-1} = \ker(H^* + I)$ is given by

$$\mathfrak{N}_{-1} = \left\{ \sum_{j=1}^{\infty} c_j \varphi_j : \{c_j\}_1^{\infty} \in l^2(\mathbb{N}) \right\}. \quad (5.3)$$

(ii) $\operatorname{dom}(H^*)$ is the direct sum of vector spaces $\operatorname{dom} H$, \mathfrak{N}_{-1} and $(-\Delta + I)^{-1} \mathfrak{N}_{-1}$, that is,

$$\begin{aligned} \operatorname{dom}(H^*) &= \{f = f_H + f_0 + (-\Delta + I)^{-1} f_1; f_H \in \operatorname{dom} H, f_0, f_1 \in \mathfrak{N}_{-1}\} \\ &= \left\{ f = f_H + \sum_{j=1}^{\infty} (\xi_{0j} \varphi_j + \xi_{1j} e_j) : f_H \in \operatorname{dom} H, \xi_0 := \{\xi_{0j}\}, \xi_1 = \{\xi_{1j}\} \in l^2(\mathbb{N}) \right\}, \end{aligned} \quad (5.4)$$

$$H^* f = -\Delta f_H - f_0 + (-\Delta)(-\Delta + I)^{-1} f_1 = -\Delta f_H + \sum_{j=1}^{\infty} (-\xi_{0j} \varphi_j + \xi_{1j} (\varphi_j - e_j/2)). \quad (5.5)$$

(iii) The triplet $\tilde{\Pi} = \{\mathcal{H}, \tilde{\Gamma}_0, \tilde{\Gamma}_1\}$, where

$$\mathcal{H} = l^2(\mathbb{N}), \quad \tilde{\Gamma}_0 f = \xi_0, \quad \tilde{\Gamma}_1 f = T_1 \xi_1, \quad f \in \operatorname{dom}(H^*), \quad (5.6)$$

is a boundary triplet for H^* .

Proof. (i): By the Sobolev embedding theorem, $f \rightarrow f(x_j)$ is a continuous linear functional on $W^{2,2}(\mathbb{R}^3)$ (see [42, Chapter 2.5]). Therefore, $\text{dom}(H) = W^{2,2}(\mathbb{R}^3) \upharpoonright \bigcap_{j=1}^{\infty} \ker(\delta_{x_j})$ is closed in the graph norm of $-\Delta$, so the operator H is closed. Since $-\Delta$ is self-adjoint, H is symmetric.

Since $d_*(X) > 0$ by assumption, Theorem 3.8 applies and shows that $\{\varphi_j\}_1^{\infty}$ is a Riesz basis of the Hilbert space \mathfrak{N}_{-1} . In particular, $n_{\pm}(H) = \infty$.

(ii): All assertions of (ii) follow from (i) and Lemma 5.1(i), applied to the self-adjoint operator $A = -\Delta$ on $L^2(\mathbb{R}^3)$. For the formula of H^*f we recall that $e_j/2 = (-\Delta + I)^{-1}\varphi_j$ and therefore, $H^*e_j = -\Delta(-\Delta + I)^{-1}\varphi_j = \varphi_j - e_j/2$.

(iii) From (3.5) it follows that $\langle \varphi_j, \varphi_k \rangle = 2^{-1}e^{-|x_j - x_k|}$, i.e., the Gram matrix of $E = \{\varphi_j\}_{j \in \mathbb{N}}$ is \mathcal{T}_1 . By Lemma 3.7, \mathcal{T}_1 defines the bounded operator T_1 on $l^2(\mathbb{N})$ with bounded inverse. Hence $\tilde{\Gamma}_0$ and $\tilde{\Gamma}_1$ are well-defined and the map $(\tilde{\Gamma}_0, \tilde{\Gamma}_1) : \text{dom}(A^*) \rightarrow \mathcal{H} \oplus \mathcal{H}$ is surjective.

Next we verify the Green formula. Let $f, g \in \text{dom}(H^*)$. By (5.4), these vectors are of the form

$$f = f_H + f_0 + (-\Delta + I)^{-1}f_1, \quad g = g_H + g_0 + (-\Delta + I)^{-1}g_1$$

with $f_H, g_H \in \text{dom } H$ and $f_0, f_1, g_0, g_1 \in \mathfrak{N}_{-1}$. By (5.3), f_0, f_1, g_0, g_1 can be written as

$$f_0 = \sum_{j=1}^{\infty} \xi_{0j} \varphi_j, \quad f_1 = \sum_{j=1}^{\infty} \xi_{1j} \varphi_j, \quad g_0 = \sum_{j=1}^{\infty} \eta_{0j} \varphi_j, \quad g_1 = \sum_{j=1}^{\infty} \eta_{1j} \varphi_j,$$

where $\{\xi_{0j}\}_{j \in \mathbb{N}}, \{\xi_{1j}\}_{j \in \mathbb{N}}, \{\eta_{0j}\}_{j \in \mathbb{N}}, \{\eta_{1j}\}_{j \in \mathbb{N}} \in l^2(\mathbb{N})$. Using the Green identity for the boundary triplet $\Pi' = (\mathcal{H}', \Gamma'_0, \Gamma'_1)$ in Lemma 5.1, applied to $A = H$ and $\tilde{A} = -\Delta$, we derive the identity

$$\begin{aligned} \langle H^*f, g \rangle - \langle f, H^*g \rangle &= \langle \Gamma'_1 f, \Gamma'_0 g \rangle - \langle \Gamma'_0 f, \Gamma'_1 g \rangle = \langle f_1, g_0 \rangle_{\mathfrak{N}_{-1}} - \langle f_0, g_1 \rangle_{\mathfrak{N}_{-1}} \\ &= \sum_{j,k=1}^{\infty} (\xi_{1j} \overline{\eta_{0k}} - \xi_{0j} \overline{\eta_{1k}}) \langle \varphi_j, \varphi_k \rangle = \sum_{k=1}^{\infty} ((T_1 \xi_1)_k \overline{\eta_{0k}} - \xi_{0k} \overline{(T_1 \eta_1)_k}) \\ &= \langle T_1 \xi_1, \eta_0 \rangle - \langle \xi_1, T_1 \eta_0 \rangle = \langle \tilde{\Gamma}_1 f, \tilde{\Gamma}_0 g \rangle_{\mathcal{H}} - \langle \tilde{\Gamma}_0 f, \tilde{\Gamma}_1 g \rangle_{\mathcal{H}}, \end{aligned}$$

which completes the proof. \square

However, we prefer to work with another boundary triplet. For this purpose we define

$$(T_0(\xi_j))_k = -\xi_k + \sum_{j \in \mathbb{N}, j \neq k} \xi_j \frac{e^{-|x_k - x_j|}}{|x_k - x_j|}, \quad \{\xi_j\}_{j \in \mathbb{N}} \in l^2(\mathbb{N}). \quad (5.7)$$

It follows from the assumption $d_*(X) > 0$ and the fact that the matrix $(2^{-1}e^{-|x_j - x_k|})_{j,k \in \mathbb{N}}$ defines a bounded operator T_1 on $l^2(\mathbb{N})$ by Lemma 3.7, that T_0 is a bounded self-adjoint operator on $l^2(\mathbb{N})$.

Next we slightly modify the boundary triplet $\tilde{\Pi} = \{\mathcal{H}, \tilde{\Gamma}_0, \tilde{\Gamma}_1\}$ and express the trace mappings $\tilde{\Gamma}_j$ in terms of the "boundary values". We abbreviate

$$\tilde{G}_{\sqrt{z}}(x) = \begin{cases} \frac{e^{i\sqrt{z}|x|}}{|x|}, & x \neq 0; \\ 0, & x = 0. \end{cases} \quad (5.8)$$

Proposition 5.3. *Let H be the Schrödinger operator defined by (3.1). Suppose that $d_*(X) > 0$.*

(i) *The triplet $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$, where $\mathcal{H} = l^2(\mathbb{N})$,*

$$\Gamma_0 f = \left\{ \lim_{x \rightarrow x_k} f(x) |x - x_k| \right\}_1^{\infty} =: \{\xi_{0k}\}_1^{\infty}, \quad \Gamma_1 f = \left\{ \lim_{x \rightarrow x_k} (f(x) - \xi_{0k} |x - x_k|^{-1}) \right\}_1^{\infty}, \quad (5.9)$$

is a boundary triplet for H^* .

(ii) The deficiency subspace $\mathfrak{N}_z = \mathfrak{N}_z(H)$ is $\mathfrak{N}_z = \left\{ \sum_{j=1}^{\infty} c_j \varphi_{j,z} : \{c_j\}_1^{\infty} \in l^2(\mathbb{N}) \right\}$, $z \in \mathbb{C} \setminus \mathbb{R}$.

(iii) The gamma field $\gamma(\cdot)$ of the triplet $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ is given by

$$\gamma(z)(\{c_j\}) = \sum_{j=1}^{\infty} c_j \varphi_{j,z}, \quad \{c_j\}_1^{\infty} \in l^2(\mathbb{N}), \quad z \in \mathbb{C} \setminus [0, +\infty). \quad (5.10)$$

(iv) The corresponding Weyl function acts by

$$(M(z)\{c_j\})_k = c_k i\sqrt{z} + \sum'_{j \in \mathbb{N}} c_j \frac{e^{i\sqrt{z}|x_k - x_j|}}{|x_k - x_j|}, \quad \{c_j\}_{j \in \mathbb{N}} \in l^2(\mathbb{N}), \quad z \in \mathbb{C} \setminus [0, +\infty), \quad (5.11)$$

that is, the operator $M(z)$ is given by the matrix

$$\mathcal{M}(z) = \left(i\sqrt{z}\delta_{jk} + \tilde{G}_{\sqrt{z}}(x_j - x_k) \right)_{j,k=1}^{\infty}. \quad (5.12)$$

Proof. (i) Since $T_0 = T_0^* \in [\mathcal{H}]$ and $\tilde{\Pi}$ is boundary triplet for H^* by Proposition 5.2(iii), so is the triplet $\Pi' = \{\mathcal{H}, \Gamma'_0, \Gamma'_1\}$, where

$$\mathcal{H} = l^2(\mathbb{N}), \quad \Gamma'_0 := \tilde{\Gamma}_0, \quad \text{and} \quad \Gamma'_1 = \tilde{\Gamma}_1 + T_0 \tilde{\Gamma}_0. \quad (5.13)$$

It therefore suffices to show that $\Gamma_j = \Gamma'_j$, $j = 0, 1$.

Let $f \in \text{dom } H^*$. By Proposition 5.2(ii), f is of the form $f = f_H + f_0 + (-\Delta + I)^{-1}f_1$, where $f_H \in \text{dom}(H)$, $f_0 = \sum_{j \in \mathbb{N}} \xi'_{0j} \varphi_j$ and $f_1 = \sum_{j \in \mathbb{N}} \xi_{1j} \varphi_j$. Then $(-\Delta + I)^{-1}f_1 = 2^{-1} \sum_j \xi_{1j} e_j$.

Fix $k \in \mathbb{N}$. Since the series $f_0 = \sum_{j \in \mathbb{N}} \xi'_{0j} \varphi_j$ converges uniformly on compact subsets of $\mathbb{R}^3 \setminus X$ and $f_H \in W^{2,2}(\mathbb{R}^3)$ is continuous and $f_H(x_j) = 0$ by (3.1), we get

$$\xi_{0k} = \lim_{x \rightarrow x_k} f(x)|x - x_k| = \xi'_{0k} = (\tilde{\Gamma}_0 f)_k = (\Gamma'_0 f)_k.$$

This proves the first formula of (5.9). The second formula is derived by

$$\begin{aligned} \lim_{x \rightarrow x_k} (f(x) - \xi_{0k}|x - x_k|^{-1}) &= \lim_{x \rightarrow x_k} \left(\xi_{0k} \frac{e^{-|x - x_k|} - 1}{|x - x_k|} + \sum_{j \neq k}^{\infty} \xi_{0j} \frac{e^{-|x - x_j|}}{|x - x_j|} + 2^{-1} \sum_{j=1}^{\infty} \xi_{1j} e^{-|x - x_j|} \right) \\ &= -\xi_{0k} + \sum_{j \neq k}^{\infty} \xi_{0j} \frac{e^{-|x_k - x_j|}}{|x_k - x_j|} + 2^{-1} \sum_{j=1}^{\infty} \xi_{1j} e^{-|x_k - x_j|} = (T_0(\xi_{0j}))_k + (T_1(\xi_{1j}))_k = (\Gamma'_1 f)_k, \end{aligned}$$

where T_0 is defined by (5.7), and T_1 is introduced in Proposition 5.2.

(ii) follows at once from Corollary 3.10.

(iii) Clearly, $\lim_{x \rightarrow x_k} (\varphi_{k,z}(x) - \varphi_k(x))|x - x_k| = 0$. Therefore, by (5.9), $\Gamma_0(\varphi_{k,z} - \varphi_k) = 0$ and so $\Gamma_0 \varphi_{k,z} = \Gamma_0 \varphi_k = e_k$, where $e_k = \{\delta_{jk}\}_{j=1}^{\infty}$ is the standard orthonormal basis of $l^2(\mathbb{N})$. Hence, by (4.5) combined with (ii), the gamma field is of the form given in (5.10).

(iv) Next we prove the formula for the Weyl function. Since M is linear and bounded, it suffices to prove this formula for the vectors e_l , $l \in \mathbb{N}$. Fix $l \in \mathbb{N}$. The function $\varphi_{l,z} \in \text{dom}(H^*)$

is of the form (5.4), i.e., $\varphi_{l,z} = f_{H,z} + f_{0,z} + (-\Delta + I)^{-1}f_{1,z}$, where $f_{0,z} = \sum_{j \in \mathbb{N}} \xi_{0j}(z)\varphi_j$ and $f_{1,z} = \sum_{j \in \mathbb{N}} \xi_{1j}(z)\varphi_j$. Then, by (5.9) and (5.1),

$$\xi_{0j}(z) = \lim_{x \rightarrow x_j} \varphi_{l,z}(x)|x-x_j| = \delta_{jl}, \quad j \in \mathbb{N}, \quad \text{i.e.,} \quad f_{0,z}(x) = |x-x_l|^{-1}e^{-|x-x_l|}, \quad (5.14)$$

so $f_{0,z}$ does not depend on z . Since $\xi_{0k}(z) = 0$ for $k \neq l$, (5.9) and (5.1) yield

$$(\Gamma_1 \varphi_{l,z})_k = \lim_{x \rightarrow x_k} (\varphi_{l,z} - \xi_{0k}|x-x_k|^{-1}) = \lim_{x \rightarrow x_k} \varphi_{l,z}(x) = \frac{e^{i\sqrt{z}|x_l-x_k|}}{|x_l-x_k|}, \quad k \neq l, \quad k, l \in \mathbb{N}.$$

Similarly, using that $\xi_{0l}(z) = 1$ it follows from (5.9) and (5.1) that $(\Gamma_1 \varphi_{l,z})_l = i\sqrt{z}$. Inserting these expressions into (4.5) with account of (5.10) we arrive at the formula (5.11) for the Weyl function. \square

Remark 5.4. (i) Statement (i) in Lemma 5.1 goes back to the paper by M.I. Vishik [55] and was systematically used in the works of M. Birman and G. Grubb [24]. Statement (ii) is contained in a slightly different form in [17, Remark 4].

(ii) Proposition 5.2(i) was obtained in [37, Lemma 4.1] for $m = 1$ and for $m < \infty$ in [4, Theorem 1.1.2]. In the case $m = \infty$ another description of $\text{dom}(H_B)$ with diagonal $B = B^*$ is contained in [4, Theorem 3.1.1.2].

(iii) For $m < \infty$ another construction of a boundary triplet for H_3^* is contained in [21, Proposition 4.1], while even in this case the proof of Proposition 5.2(iii) is simpler. In the case $m = 1$ other constructions can be found in [37, Theorem 2.1], [14] and [27].

Another construction of a boundary triplet for general elliptic operators with boundary conditions on a set of zero Lebesgue measure can be found in [32]. However this construction does not allow to compute the Weyl function and obtain other spectral results.

(iv) In the case $m < \infty$ the Weyl function in the form (5.12) appeared in [4, chapter II.1]. In this connection we also mention the paper by Posilicano [45, Example 5.3]. In the case $m = 1$ the Weyl function was also computed by another method in [9, Section 10.3].

5.2 Some spectral properties of self-adjoint realizations

In this subsection we apply the theory of boundary triplets to describe and study self-adjoint extensions of the minimal Schrödinger operator H of the form (3.1).

Proposition 5.5. *Let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ the boundary triplet for H^* defined in Proposition 5.3 (see (5.9)). Let T_0 be defined by (5.7) and $T_1 = 2^{-1}(e^{-|x_j-x_k|})_{j,k \in \mathbb{N}}$. Then:*

(i) *The set of self-adjoint realizations $\tilde{H} \in \text{Ext}_H$ is parameterized by the set of linear relations $\Theta = \Theta^* \in \tilde{\mathcal{C}}(\mathcal{H})$ as follows: $H_\Theta = H^* \upharpoonright \text{dom}(H_\Theta)$, where*

$$\text{dom}(H_\Theta) = \left\{ f = f_H + \sum_{j=1}^{\infty} \left(\xi_{0j} \frac{e^{-|x-x_j|}}{|x-x_j|} + \xi_{1j} e^{-|x-x_j|} \right) : f_H \in \text{dom}(H), (\xi_0, T_0 \xi_0 + T_1 \xi_1) \in \Theta \right\}. \quad (5.15)$$

Moreover, we have $\Theta = \Theta_{op} \oplus \Theta_\infty$ where Θ_{op} is the graph of an operator $B = B^*$ in $\mathcal{H}_0 := \overline{\text{dom}(\Theta)}$ and Θ_∞ is the multivalued part of Θ , and $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_\infty$, where $\mathcal{H}_\infty := \text{mul}(\Theta)$ and

$$\Theta_\infty := \{0, \mathcal{H}_\infty\} := \{\{0, T_1 \xi_1''\} : \xi_1'' \perp T_1 \xi_0, \xi_0 \in \mathcal{H}_0\}, \quad (5.16)$$

$$\Theta_{op} = \{\{\xi_0, T_0 \xi_0 + T_1 \xi_1'\} : \xi_0 \in \mathcal{H}_0, \xi_1' = T_1^{-1}(B \xi_0 - T_0 \xi_0)\}. \quad (5.17)$$

In particular, $\tilde{H} = H_\Theta$ is disjoint with H_0 if and only if $\overline{\text{dom}(\Theta)} = \mathcal{H} = l^2(\mathbb{N})$. In this case $\Theta = \Theta_{op}$ is the graph of B , so that $H_\Theta = H^* \upharpoonright (\ker(\Gamma_1 - B\Gamma_0))$.

(ii) Let $z \in \mathbb{C} \setminus \overline{\mathbb{R}}_+$. Then $z \in \sigma_p(H_\Theta)$ if and only if $0 \in \sigma_p\left(\Theta - (i\sqrt{z}\delta_{jk} + \tilde{G}_{\sqrt{z}}(x_j - x_k))_{j,k=1}^\infty\right)$. The corresponding eigenfunctions ψ_z have the form

$$\psi_z = \sum_{j=1}^\infty \xi_j |x - x_j|^{-1} e^{i\sqrt{z}|x-x_j|}, \quad \text{where} \quad (\xi_j) \in \ker(\Theta - M(z)) \subset l^2(\mathbb{N}). \quad (5.18)$$

(iii) The resolvent of the extension $-\Delta_{\Theta,X} := H_\Theta$ admits the integral representation

$$((-\Delta_{\Theta,X} - z)^{-1}f)(x) = \int_{\mathbb{R}^3} T_{\Theta,X}(x, y; z) f(y) dy, \quad z \in \rho(-\Delta_{\Theta,X}), \quad (5.19)$$

with kernel $T_{\Theta,X}(\cdot, \cdot; z)$ defined by

$$T_{\Theta,X}(x, y; z) = \frac{e^{i\sqrt{z}|x-y|}}{4\pi|x-y|} + \sum_{j,k} \Theta_{jk}(z) \frac{e^{i\sqrt{z}|y-x_j|}}{|y-x_j|} \cdot \frac{e^{i\sqrt{z}|x-x_k|}}{|x-x_k|}, \quad (5.20)$$

where $(\Theta_{jk}(z))_{j,k \in \mathbb{N}}$ is the matrix representation of the operator $(\Theta - M(z))^{-1}$ on $l^2(\mathbb{N})$.

Proof. (i) Formula (5.15) is immediate from Proposition 4.6, formula (4.3).

Both formulas (5.16) and (5.17) are proved by direct computations. We show that (5.16) and (5.17) imply the self-adjointness of Θ ; the proof of the converse implication is similar. Indeed, it follows from (5.16) and (5.17) that $(T_1\xi_1'', \xi_0) = 0 = (\xi_0, T_1\xi_1'')$ and

$$(T_1\xi_1', \xi_0) = (B\xi_0 - T_0\xi_0, \xi_0) = (\xi_0, B\xi_0 - T_0\xi_0) = (\xi_0, T_1\xi_1'). \quad (5.21)$$

Hence we have $(T_1\xi_1, \xi_0) = (\xi_0, T_1\xi_1)$ for all $(\xi_0, \xi_1) \in \Theta$. It is easily checked that the latter condition is equivalent to the self-adjointness of the relation Θ .

(ii) The symmetric operator H is in general not simple. It admits a direct sum decomposition $H = \hat{H} \oplus H'$ where \hat{H} is a simple symmetric operator and H' is self-adjoint. Define $\hat{\Pi} = \{\mathcal{H}, \hat{\Gamma}_0, \hat{\Gamma}_1\}$, where $\hat{\Gamma}_j := \Gamma_j \upharpoonright \text{dom}(\hat{H}^*)$, $j \in \{0, 1\}$. Clearly, $\hat{\Pi}$ is a boundary triplet for \hat{H}^* and the corresponding Weyl function $\hat{M}(\cdot)$ coincides with the Weyl function $M(\cdot)$ of Π . Further, any proper extension $\tilde{H} = H_\Theta$ of H admits a decomposition $H_\Theta = \hat{H}_\Theta \oplus H'$. Being a part of H_0 , the operator H' is non-negative. Therefore, for $z \in \mathbb{C} \setminus \overline{\mathbb{R}}_+$, we have $z \in \sigma_p(H_\Theta)$ if and only if $z \in \sigma_p(\hat{H}_\Theta)$. Thus, it suffices to prove the assertion for extensions \hat{H}_Θ of the *simple symmetric operator* \hat{H} . But then the statement follows from Propositions 4.8 and 5.3(ii) and formula (5.10).

(iii) Noting that $i\sqrt{z} = \overline{i\sqrt{z}}$ it follows from (5.1) that $\varphi_{j,\bar{z}} = \overline{\varphi_{j,z}}$. Therefore, (5.10) implies that

$$\gamma^*(\bar{z})f = \sum_{k=1}^\infty \left(\int_{\mathbb{R}^3} f(x) \overline{\varphi_{k,\bar{z}}(x)} dx \right) e_k = \sum_{k=1}^\infty \left(\int_{\mathbb{R}^3} f(x) \frac{e^{i\sqrt{z}|x-x_k|}}{|x-x_k|} dx \right) e_k, \quad (5.22)$$

where $e_k = \{\delta_{jk}\}_{j=1}^\infty$ is the standard basis of $l^2(\mathbb{N})$.

Inserting (5.22) and (5.10) into the Krein type formula (4.6) and applying the formula (3.2) for the resolvent of the free Hamiltonian $-\Delta$, we obtain

$$((-\Delta_{\Theta,X} - z)^{-1}f)(x) = \int_{\mathbb{R}^3} \frac{e^{i\sqrt{z}|x-y|}}{4\pi|x-y|} f(y) dy + \sum_{j,k} [(\Theta - M(z))^{-1}]_{j,k} (f, \overline{\varphi_{k,z}}) \varphi_{j,z}(x).$$

Clery, the latter is equivalent to the representations (5.19)–(5.20). \square

Next we turn to nonnegative or lower semibounded self-adjoint extensions of H . For this we need the following technical result.

Lemma 5.6. *Retain the assumptions of Proposition 5.3 and let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be the boundary triplet for H^* defined therein. Then:*

(i) *There exists a lower semibounded self-adjoint operator $M(0)$ on $\mathcal{H} = l^2(\mathbb{N})$ which is the limit of $M(-x)$ in the strong resolvent convergence as $x \rightarrow +0$.*

(ii) *The quadratic form $\mathbf{t}_{M(0)}$ of $M(0)$ is given by*

$$\mathbf{t}_{M(0)}[\xi] = \sum_{|j-k|>0} \frac{1}{|x_j - x_k|} \xi_j \bar{\xi}_k, \quad \text{dom}(\mathbf{t}_{M(0)}) = \left\{ \xi = \{\xi_j\} \in l^2(\mathbb{N}) : \sum_{|j-k|>0} \frac{1}{|x_j - x_k|} \xi_j \bar{\xi}_k < \infty \right\}. \quad (5.23)$$

(iii) *The operator $M(0) = M(0)^*$ associated with the form $\mathbf{t}_{M(0)}$ is uniquely determined by the following conditions: $\text{dom}(M(0)) \subset \text{dom}(\mathbf{t}_{M(0)})$ and*

$$(M(0)\xi, \eta) = \sum_{|j-k|>0} \frac{1}{|x_j - x_k|} \xi_j \bar{\eta}_k, \quad \xi = \{\xi_j\} \in \text{dom}(M(0)), \quad \eta = \{\eta_j\} \in \text{dom}(\mathbf{t}_{M(0)}). \quad (5.24)$$

(iv) *If, in addition, $\sum'_{j \in \mathbb{N}} |x_j - x_k|^{-2} < \infty$ for every $k \in \mathbb{N}$, then $e_k \in \text{dom}(M(0))$, $k \in \mathbb{N}$, where $e_k = \{\delta_{jk}\}_{j=1}^\infty$ is the standard orthonormal basis of $l^2(\mathbb{N})$, and the matrix*

$$\mathcal{M}'(0) := \left(\frac{1 - \delta_{kj}}{|x_k - x_j| + \delta_{kj}} \right)_{j,k=1}^\infty, \quad (5.25)$$

defines a (minimal) closed symmetric operator $M'(0)$ on $l^2(\mathbb{N})$. Moreover,

$$\text{dom}(M'(0)^*) = \left\{ \{\xi_j\} \in l^2(\mathbb{N}) : \sum_{j \in \mathbb{N}} \left| \sum'_{k \in \mathbb{N}} |x_j - x_k|^{-1} \xi_k \right|^2 < \infty \right\}. \quad (5.26)$$

(v) *The operator $M'(0)$ is semibounded from below and its Friedrichs extension $M'(0)_F$ coincides with $M(0)$, that is, $M'(0)_F = M(0)$.*

Proof. (i) The assertion follows by combining Propositions 4.10(i) and 5.3(iv) (cf. formulas (5.12) and (5.8)).

(ii) By Proposition 4.10(i),

$$\mathbf{t}_{M(0)}[\xi] := \lim_{t \downarrow 0} (M(-t)\xi, \xi), \quad \xi \in \text{dom}(\mathbf{t}_{M(0)}) := \left\{ \eta : \lim_{t \downarrow 0} (M(-t)\eta, \eta) < \infty \right\}. \quad (5.27)$$

Let us denote for the moment the form defined in (5.23) by \mathbf{t}_0 . We have to show that $\mathbf{t}_0 = \mathbf{t}_{M(0)}$.

Note that the function $f(t) = (1 - e^{-t})/t = \int_0^1 e^{-st} ds$ is absolutely monotone, $f \in M[0, \infty)$. Hence $f \in \Phi_3$. This fact together with (5.12) and (5.23) yields

$$\mathbf{t}_0[\xi] - (M(-t)\xi, \xi) = \sum_{|k-j|>0} \frac{1 - e^{-t|x_j - x_k|}}{|x_j - x_k|} \xi_j \bar{\xi}_k > 0, \quad t > 0, \quad \xi = \{\xi_j\}_1^\infty \in \text{dom}(\mathbf{t}_0). \quad (5.28)$$

Thus, for any $\xi \in \text{dom}(\mathbf{t}_0)$ the limit $\lim_{t \downarrow 0} (M(-t)\xi, \xi)$ is finite and by (5.27), $\text{dom}(\mathbf{t}_0) \subset \text{dom}(\mathbf{t}_{M(0)})$.

Now we prove that $\mathbf{t}_{M(0)}[\xi] = \mathbf{t}_0[\xi]$ for all $\xi \in \text{dom}(\mathbf{t}_0)$. For finite vectors this follows at once from (5.28) and (5.27). Fix $\xi \in \text{dom}(\mathbf{t}_0)$. Given $\varepsilon > 0$ it follows from (5.23) and (5.27) that there exists $N \in \mathbb{N}$ such that the finite vector $\xi^{(N)} := \{\xi_j\}_1^N$ satisfies

$$|\mathbf{t}_0[\xi] - \mathbf{t}_0[\xi^{(N)}]| < \varepsilon \quad \text{and} \quad |\mathbf{t}_{M(0)}[\xi] - \mathbf{t}_{M(0)}[\xi^{(N)}]| < \varepsilon.$$

Then $|\mathbf{t}_0[\xi] - \mathbf{t}_{M(0)}[\xi]| < 2\varepsilon$. Since $\varepsilon > 0$ was arbitrary, this implies that $\mathbf{t}_{M(0)}[\xi] = \mathbf{t}_0[\xi]$.

The equality $\text{dom}(\mathbf{t}_0) = \text{dom}(\mathbf{t}_{M(0)})$ is obvious.

(iii) follows from (ii) and the first form representation theorem (cf. [31, Theorem 6.2.1]).

(iv) By the assumption $\sum_{j \in \mathbb{N}} |x_j - x_k|^{-2} < \infty$, we have $e_k \in \text{dom}(M(0))$. Now [2, Theorem 56.4] gives the first assertion, while the second follows from [2, Theorem 56.2].

(v) Define a quadratic form \mathbf{t}'_0 by $\mathbf{t}'_0[\xi] := (M'(0)\xi, \xi)$, $\xi \in \text{dom}(\mathbf{t}'_0) = \text{dom}(M'(0))$. Clearly, the finite vectors are dense in $\text{dom}(\mathbf{t}_{M(0)})$ with respect to the norm $\|\xi\|_+^2 := \mathbf{t}_{M(0)}[\xi] + C\|\xi\|^2$ for sufficiently large $C > 0$. Since $\mathbf{t}'_0[\eta] = \mathbf{t}_{M(0)}[\eta]$, the closure of the form \mathbf{t}'_0 is $\mathbf{t}_{M(0)}$. Since $M(0) = M(0)^*$ and $\text{dom}(M(0)) \subset \text{dom} \mathbf{t}_{M(0)}$, this completes the proof. \square

Remark 5.7. As above, let $f(t) = (1 - e^{-t})/t$. By Theorem 2.10, $f(| \cdot |)$ is strictly X -positive definite, hence the quadratic form $\mathbf{t}_0 - \mathbf{t}_{M(-t)}$ in (5.28) is strictly positive definite. However, note that this form is bounded from above if and only if $M(0)$ is bounded. The latter depends on the set X and shows that the assumption (2.14) in Theorem 2.10 is essential.

Theorem 5.8. *Let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be the boundary triplet for H^* defined in Proposition 5.3, M the corresponding Weyl function and let Θ be a self-adjoint relation on \mathcal{H} . Then*

(i) *The operator $H_0 := H^* \upharpoonright \ker \Gamma_0$ is the free Laplacian $H_0 = -\Delta$, $\text{dom}(H_0) = \text{dom}(\Delta) = W^{2,2}(\mathbb{R}^3)$. Moreover, H_0 is the Friedrichs extension H_F of H and $\text{dom}(\mathbf{t}_{H_0}) = W^{1,2}(\mathbb{R}^3)$.*

(ii) *The operator $H_{M(0)}$ is the Krein extension H_K of H and given by $H_K = H^* \upharpoonright \text{dom}(H_K)$, where the domain $\text{dom}(H_K)$ is the direct sum of $\text{dom}(H)$ and the vector space*

$$\left\{ \sum_{j=1}^{\infty} (\xi_{0j} \varphi_j + \xi_{1j} e_j) : \{\xi_{1j}\} = T_1^{-1}(M(0) - T_0)\xi_0, \quad \{\xi_{0j}\} \in \text{dom}(M(0)) \right\}.$$

The extensions $H_0 = H_F$ and H_K are disjoint. They are transversal if and only if the operator $M(0)$ is bounded on $l^2(\mathbb{N})$. For instance, this is true whenever condition (2.33) is satisfied.

(iii) *$H_\Theta \geq 0$ if and only if Θ is semibounded below, $\text{dom}(\mathbf{t}_\Theta) \subset \text{dom}(\mathbf{t}_{M(0)})$ and $\mathbf{t}_\Theta \geq \mathbf{t}_{M(0)}$.*

In particular, $H_\Theta \geq 0$ when $\text{dom}(\Theta) \subset \text{dom}(M(0))$ and $\Theta - M(0) \geq 0$.

(iv) *H_Θ is lower semibounded if and only if Θ is. In this case the quadratic form \mathbf{t}_{H_Θ} is*

$$\text{dom}(\mathbf{t}_{H_\Theta}) = W^{1,2}(\mathbb{R}^3) \dot{+} \left\{ \sum_{j=1}^{\infty} \xi_j \varphi_j : \xi = \{\xi_j\}_{j \in \mathbb{N}} \in \text{dom}(\mathbf{t}_\Theta) \subset l^2(\mathbb{N}) \right\}, \quad (5.29)$$

$$\mathbf{t}_{H_\Theta}[f] + \|f\|_{L^2}^2 = \int_{\mathbb{R}^3} (|\nabla g(x)|^2 + |g(x)|^2) dx + \mathbf{t}_\Theta[\xi] - \sum_{|k-j|>0} \frac{e^{-|x_j-x_k|}}{|x_j-x_k|} \xi_j \bar{\xi}_k, \quad (5.30)$$

where $f = g + \sum_{j \in \mathbb{N}} \xi_j \varphi_j \in \text{dom}(\mathbf{t}_{H_\Theta})$ with $g \in W^{1,2}(\mathbb{R}^3)$ and $\xi = \{\xi_j\}_{j \in \mathbb{N}} \in \text{dom}(\mathbf{t}_\Theta)$.

(v) *In particular, for the quadratic form $\mathbf{t}_{H_K} = \mathbf{t}_{H_{M(0)}}$ we have*

$$\text{dom}(\mathbf{t}_{H_K}) = W^{1,2}(\mathbb{R}^3) \dot{+} \left\{ \sum_{j=1}^{\infty} \xi_j \varphi_j : \{\xi_j\}_1^\infty \in l^2(\mathbb{N}), \sum_{|k-j|>0} |x_j - x_k|^{-1} \xi_j \bar{\xi}_k < \infty \right\}, \quad (5.31)$$

$$\mathbf{t}_{H_K}[f] + \|f\|_{L^2}^2 = \int_{\mathbb{R}^3} |\nabla g(x)|^2 dx + \|g\|_{L^2}^2 + \sum_{|k-j|>0} \frac{1 - e^{-|x_j-x_k|}}{|x_j-x_k|} \xi_j \bar{\xi}_k, \quad (5.32)$$

where $f = g + \sum_{j \in \mathbb{N}} \xi_j \varphi_j \in \text{dom}(\mathbf{t}_{H_{M(0)}})$ with $g \in W^{1,2}(\mathbb{R}^3)$ and $\{\xi_j\}_{j \in \mathbb{N}} \in \text{dom}(\mathbf{t}_{M(0)})$.

(vi) If Θ is lower semibounded and $\text{dom}(\mathbf{t}_\Theta) \subset \text{dom}(\mathbf{t}_{M(0)})$, then $\kappa_-(H_\Theta) = \kappa_-(\mathbf{t}_{\Theta-M(0)})$.

If, in addition, $\text{dom}(\Theta) \subset \text{dom}(M(0))$, then $\kappa_-(H_\Theta) = \kappa_-(\Theta - M(0))$.

(vii) If $M(0)$ is bounded, i.e. H_K and H_F are transversal, we have the implication

$$(\Theta - M(0))E_{\Theta-M(0)}(-\infty, 0) \in \mathfrak{S}_p(\mathcal{H}) \implies H_\Theta E_{H_\Theta}(-\infty, 0) \in \mathfrak{S}_p(\mathfrak{H}). \quad (5.33)$$

For instance, implication (5.33) holds whenever condition (2.33) is satisfied.

Proof. (i) The first statement is immediate from (5.4) and definition (5.9) of Γ_0 .

Further, integrating by parts one gets

$$\mathbf{t}_H[f] + \|f\|_{L^2}^2 := (Hf, f) + \|f\|_{L^2}^2 = \int_{\mathbb{R}^3} |\nabla f(x)|^2 dx + \|f\|_{L^2}^2 =: \|f\|_{W^{1,2}}^2, \quad f \in \text{dom}(H). \quad (5.34)$$

Since $\text{dom}(H)$ is dense in $W^{1,2}(\mathbb{R}^3)$, the closure \mathbf{t}_H of \mathbf{t}'_H is defined by (5.34) on the domain $\text{dom}(\mathbf{t}_H) = W^{1,2}(\mathbb{R}^3)$. Noting that $\text{dom}(\mathbf{t}_{H_0}) = W^{1,2}(\mathbb{R}^3) = \text{dom}(\mathbf{t}_H)$ we get the result.

We present another proof that is based on the Weyl function. It follows from (5.12) and (5.8) that $\lim_{x \downarrow -\infty} (M(x)h, h) = -\infty$ for $h \in \mathcal{H} \setminus \{0\}$. It remains to apply Proposition 4.10(iii).

(ii) By Proposition 4.10, $\text{dom}(H_K) = \ker(\Gamma_1 - M(0)\Gamma_0)$ since H_K and $H_0 = H_F$ are disjoint. Inserting the expressions from (5.9) and (5.13) for Γ_1 and Γ_0 we get the result.

(iii) follows immediately from Proposition 4.12(i).

(iv): Let $\xi = \{\xi_j\}_1^\infty \in l^2(\mathbb{N})$. Set $|\xi| := \{|\xi_j|\}_{j \in \mathbb{N}}$. Then we derive from (5.12)

$$\begin{aligned} |\langle M(-t^2)\xi, \xi \rangle + \frac{t}{4\pi} \|\xi\|_{l^2}^2| &\leq \left| \sum_{|k-j|>0} \frac{e^{-t|x_j-x_k|}}{|x_j-x_k|} \xi_j \bar{\xi}_k \right| \leq \frac{1}{d_*(X)} \sum_{j,k \in \mathbb{N}} e^{-t|x_j-x_k|} |\xi_j \bar{\xi}_k| \\ &\leq d_*(X)^{-1} e^{-(t-1)d_*(X)} \sum_{j,k \in \mathbb{N}} e^{-|x_j-x_k|} |\xi_j \bar{\xi}_k| \\ &= d_*(X)^{-1} e^{-(t-1)d_*(X)} 2 \left| \langle T_1 |\xi|, |\xi| \rangle_{l^2(\mathbb{N})} \right| \\ &\leq d_*(X)^{-1} e^{(1-t)d_*(X)} 2 \cdot \|T_1\| \cdot \|\xi\|_{l^2(\mathbb{N})}^2. \end{aligned} \quad (5.35)$$

For any $\varepsilon > 0$, $\varepsilon < \|T_1\| d_*(X)^{-1}$, we define $t_0 = t_0(\varepsilon)$ by

$$t_0 = t_0(\varepsilon) = 1 - \ln(\varepsilon d_*(X) \|T_1\|^{-1}). \quad (5.36)$$

Then it follows from (5.35) that

$$(M(-t^2)\xi, \xi) \geq -\left(\frac{t}{4\pi} + \varepsilon\right) \|\xi\|_{l^2}^2, \quad t \geq t_0, \quad (5.37)$$

and hence $M(-t^2) \rightrightarrows -\infty$. Now Proposition 4.11 yields the first assertion.

Next we prove the second statement. By [38, Theorem 1], the domain $\text{dom}(\mathbf{t}_{H_\Theta})$ is a direct sum

$$\text{dom}(\mathbf{t}_{H_\Theta}) = \text{dom}(\mathbf{t}_H) \dot{+} \gamma(-\varepsilon^2) \text{dom}(\mathbf{t}_\Theta), \quad \varepsilon > 0. \quad (5.38)$$

Hence any $f \in \text{dom}(\mathbf{t}_{H_\Theta})$ can be written as $f = g + \gamma(-\varepsilon^2)h$, where $g \in \text{dom}(\mathbf{t}_H)$ and $h \in \text{dom}(\mathbf{t}_\Theta)$. Noting that $\text{dom}(\mathbf{t}_H) = W^{1,2}(\mathbb{R}^3)$, and combining (5.38) with (5.10) yields (5.29).

Further, by [38, Theorem 1] we have the equality

$$\mathbf{t}_{H_\Theta}[f] + \|f\|^2 = \mathbf{t}_H[g] + \|g\|^2 + \mathbf{t}_\Theta[h] - (M(-1)h, h), \quad f := g + \gamma(-1)h. \quad (5.39)$$

Using Proposition 5.3(iv) and the equality $\mathbf{t}_H[g] = \int_{\mathbb{R}^3} |\nabla g(x)|^2 dx$ we obtain (5.30).

(v) follows from (iv) with $\Theta = M(0)$.

(vi) By (i), $H_0 = H_F$. Hence the assertion is immediate from Proposition 4.12(ii).

(vii) Since H_0 is the Friedrichs extension of H , [38, Theorem 3] implies the assertion. \square

Remark 5.9. It follows from (5.31) and (5.4) that the inclusion

$$\text{dom}(\mathbf{t}_{H_K}) = W^{1,2}(\mathbb{R}^3) \dot{+} \gamma(-1) \text{dom } \mathbf{t}_{M(0)} \supset W^{2,2}(\mathbb{R}^3) \dot{+} \mathfrak{N}_{-1} = \text{dom}(H^*) \quad (5.40)$$

holds if and only if the operator $M(0)$ is bounded. This fact illustrates the following general result: for any non-negative operator A the inclusion $\text{dom}(\mathbf{t}_{A_K}) \supset \text{dom}(A^*)$ holds if and only if A_K and A_F are transversal (see [38, Remark 3]).

Remark 5.10. (i) The Krein type formula (5.19)-(5.20) was established in [4, Theorem 3.1.1.1] for a special family $H_{X,\alpha}^{(3)}$ of self-adjoint extensions by approximation method. In our notation this family is parameterized by the set of self-adjoint diagonal matrices $B_\alpha = \text{diag}(\alpha_1, \dots, \alpha_m, \dots)$. In this case

$$H_{X,\alpha}^{(3)} = H^* \upharpoonright \left\{ f = f_H + \sum_{j=1}^{\infty} \xi_{0j} \frac{e^{-|x-x_j|}}{|x-x_j|} + \sum_{k,j=1}^{\infty} b_{jk}(\alpha) \xi_{0k} e^{-|x-x_j|} \right\}, \quad (5.41)$$

where $\tilde{B}_\alpha = (b_{jk}(\alpha))_{j,k=1}^{\infty} = T_1^{-1}(B_\alpha - T_0)$. It is proved in [4, Theorem 3.1.1.1] that $H_{X,\alpha}^{(3)}$ is self-adjoint. Other parameterizations of the set of self-adjoint realizations are also contained in [32] (see also the references therein) and [44, Example 3.4]. Another version of formula (5.19)-(5.20) as well as an abstract Krein-like formula for resolvents can also be found in [44].

(ii) In the case of finitely many point interactions ($m < \infty$) different descriptions of non-negative realizations has been obtained in [8, 27, 21].

(iii) In connection with Theorem 5.8(iv) we mention the papers [34] and [26] where similar statements have been obtained for realizations of 1D Schrödinger operators (1.1) with $d_*(X) \geq 0$ and elliptic operators in exterior domains, respectively.

5.3 Ac-spectrum of self-adjoint extensions

Theorem 5.11. *Let $d_*(X) > 0$ and let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be the boundary triplet for H^* defined in Proposition 5.3. Suppose that Θ is a self-adjoint relation on \mathcal{H} . Then*

(i) *For any $p \in (0, \infty]$ we have the following equivalence:*

$$(H_\Theta - i)^{-1} - (H_0 - i)^{-1} \in \mathfrak{S}_p(\mathfrak{H}) \iff (\Theta - i)^{-1} \in \mathfrak{S}_p(\mathcal{H}). \quad (5.42)$$

(ii) *If $(\Theta - i)^{-1} \in \mathfrak{S}_1(\mathcal{H})$, then the non-negative ac-part $H_\Theta^{ac} = H_\Theta^{ac} E_{H_\Theta}(\overline{\mathbb{R}}_+)$ of the operator $H_\Theta = H_\Theta^*$ is unitarily equivalent to the Laplacian $-\Delta$.*

(iii) *Suppose that $(\Theta - i)^{-1} \in \mathfrak{S}_\infty(\mathcal{H})$ and condition (2.33) is satisfied, i.e.,*

$$C_1 := \sup_{j \in \mathbb{N}} \sum'_{k \in \mathbb{N}} \frac{1}{|x_k - x_j|} < \infty. \quad (5.43)$$

Then the ac-part $H_\Theta^{ac} = H_\Theta^{ac} E_{H_\Theta}(\overline{\mathbb{R}}_+)$ of H_Θ is unitarily equivalent to the Laplacian $-\Delta$.

Proof. (i) This assertion follows at once from Proposition 4.9.

(ii) By Proposition 5.8(i) $H_0 = -\Delta$. Therefore, by (5.42) with $p = 1$, $[(H_\Theta - i)^{-1} - (-\Delta - i)^{-1}] \in \mathfrak{S}_1(\mathfrak{H})$. It remains to apply the Kato-Rosenblum theorem (see [31]).

(iii) Let $z = t + iy \in \mathbb{C}_+$, $t > 0$, and $\sqrt{z} = \alpha + i\beta$. Clearly, $\alpha > 0, \beta > 0$ and $i\sqrt{z} = i\alpha - \beta$. It follows from (5.8) that

$$\tilde{G}_{\sqrt{z}}(|x_j - x_k|) = \frac{|e^{(-\beta + i\alpha)|x_j - x_k|}|}{|x_j - x_k|} = \frac{e^{-\beta|x_j - x_k|}}{|x_j - x_k|}, \quad j \neq k. \quad (5.44)$$

It follows from (5.12) combined with (5.43) and (5.44) that

$$\begin{aligned} \|M(t + iy)\| &\leq \sqrt{\alpha^2 + \beta^2} + e^{-\beta} \sup_{j \in \mathbb{N}} \sum'_{k \in \mathbb{N}} \frac{1}{|x_k - x_j|} \\ &= \sqrt{\alpha^2 + \beta^2} + C_1 e^{-\beta} \leq \sqrt{t} + 1 + C_1, \quad y \in [0, 1]. \end{aligned}$$

Thus, for any fixed $t > 0$ the family $M(t + iy)$ is uniformly bounded for $y \in (0, 1]$, hence the weak limit $M(t + i0) := w - \lim_{y \downarrow 0} M(t + iy)$ exists and

$$w - \lim_{y \downarrow 0} M(t + iy) =: M(t + i0) =: M(t) = i\sqrt{t}I + \left(\tilde{G}_{\sqrt{t}}(|x_j - x_k|)\right)_{j,k=1}^\infty. \quad (5.45)$$

From (5.42), applied with $p = \infty$, we conclude that $[(H_\Theta - z)^{-1} - (H_0 - z)^{-1}] \in \mathfrak{S}_\infty(\mathfrak{H})$ since $(\Theta - i)^{-1} \in \mathfrak{S}_\infty(\mathcal{H})$. To complete the proof it suffices to apply [41, Theorem 4.3] to H_Θ and $H_0 = -\Delta$. \square

To prove the next result we need the following auxiliary lemma which is of interest in itself.

Lemma 5.12. *Suppose that A is a simple symmetric operator in \mathfrak{H} and $\{\mathcal{H}, \Gamma_0, \Gamma_1\}$ is a boundary triplet for A^* with Weyl function M . Assume that for any $t \in (\alpha, \beta)$ the uniform limit*

$$M(t) := M(t + i0) := u - \lim_{y \downarrow 0} M(t + iy) \quad (5.46)$$

exists and $0 \in \rho(M_I(t))$ for $t \in (\alpha, \beta)$. Then the spectrum of any self-adjoint extension \tilde{A} of A on \mathfrak{H} in the interval (α, β) is purely absolutely continuous, i.e.,

$$\sigma_s(\tilde{A}) \cap (\alpha, \beta) = \emptyset. \quad (5.47)$$

The operator $\tilde{A}E_{\tilde{A}}(\alpha, \beta) = \tilde{A}^{ac}E_{\tilde{A}}(\alpha, \beta)$ is unitarily equivalent to $A_0E_{A_0}(\alpha, \beta)$, where $A_0 = A^ \upharpoonright \ker \Gamma_0$.*

Proof. Without loss of generality we can assume that the extensions \tilde{A} and A_0 are disjoint. Then, by Proposition 4.6(iii), there is a self-adjoint operator B on \mathcal{H} such that $\tilde{A} = A_B$, where $A_B = A^* \upharpoonright \ker(\Gamma_1 - B\Gamma_0)$.

We set $M_B(t + iy) := (B - M(t + iy))^{-1}$ and note that

$$\operatorname{Im}(M_B(t + iy)) = (B - M(t + iy))^{-1} \operatorname{Im}(M(t + iy))(B - M^*(t + iy))^{-1}, \quad y \in \mathbb{R}_+. \quad (5.48)$$

Fix $t \in (\alpha, \beta)$. By assumption we have $0 \in \rho(M_I(t))$, i.e., there exists $\varepsilon = \varepsilon(t)$ such that

$$\langle M_I(t)h, h \rangle \geq \varepsilon \|h\|^2, \quad h \in \mathcal{H}. \quad (5.49)$$

It follows from (5.46) that there exists $y_0 \in \mathbb{R}_+$ such that

$$\|M_I(t + iy) - M_I(t)\| \leq \varepsilon/2 \quad \text{for } y \in [0, y_0]. \quad (5.50)$$

Combining (5.49) with (5.50) we get

$$\begin{aligned} \langle M_I(t + iy)h, h \rangle &= \langle M_I(t)h, h \rangle + \langle (M_I(t + iy) - M_I(t))h, h \rangle \\ &\geq 2^{-1}\varepsilon\|h\|^2, \quad y \in [0, y_0]. \end{aligned}$$

Hence, for any $h \in \text{dom}(B)$,

$$\begin{aligned} \|(M(t + iy) - B)h\| \cdot \|h\| &\geq |\langle (M(t + iy) - B)h, h \rangle| \\ &\geq \text{Im}\langle (M(t + iy) - B)h, h \rangle = \langle M_I(t + iy)h, h \rangle \geq 2^{-1}\varepsilon\|h\|^2, \quad y \in [0, y_0]. \end{aligned}$$

Since $0 \in \rho(M(t + iy) - B)$, the latter inequality is equivalent to

$$\|(M(t + iy) - B)^{-1}\| \leq 2\varepsilon^{-1}, \quad y \in [0, y_0]. \quad (5.51)$$

It follows that

$$\begin{aligned} &\|(B - M(t + iy))^{-1} - (B - M(t))^{-1}\| \\ &= \|(B - M(t + iy))^{-1}[M(t + iy) - M(t)](B - M(t))^{-1}\| \\ &\leq 4\varepsilon^{-2}\|M(t + iy) - M(t)\|, \quad y \in [0, y_0]. \end{aligned}$$

Hence

$$u - \lim_{y \downarrow 0} (B - M(t + iy))^{-1} = (B - M(t))^{-1}. \quad (5.52)$$

Next, it is easily seen that $\Pi_B = \{\mathcal{H}, \Gamma_0^B, \Gamma_1^B\}$, where $\Gamma_0^B = B\Gamma_0 - \Gamma_1$, $\Gamma_1^B = \Gamma_0$, is a generalized boundary triplet for $A_* \subset A^*$, $\text{dom}(A_*) = \text{dom}(A_0) + \text{dom}(A_B)$ (see [17] for the definitions). The corresponding Weyl function is $M_B(\cdot) = (B - M(\cdot))^{-1}$. Therefore, combining (5.52) with [13, Theorem 4.3], we get $\tau_s(A_B) \cap (\alpha, \beta) = \emptyset$, i.e., $\tilde{A}E_{\tilde{A}}(\alpha, \beta) = \tilde{A}^{ac}E_{\tilde{A}}(\alpha, \beta)$.

Moreover, passing to the limit in (5.48) as $y \downarrow 0$, and using (5.46) and (5.52), we obtain

$$\text{Im}(M_B(t + i0)) = (B - M(t + i0))^{-1}M_I(t + i0)(B - M^*(t + i0))^{-1}, \quad t \in (\alpha, \beta). \quad (5.53)$$

Since $\ker(B - M^*(t + i0))^{-1} = \{0\}$, we have

$$\text{rank}(\text{Im}(M_B(t + i0))) = \text{rank}(\text{Im}(M_I(t + i0))), \quad t \in (\alpha, \beta). \quad (5.54)$$

By Proposition 4.14 the operators $A_BE_{A_B}(\alpha, \beta)$ and $A_0E_{A_0}(\alpha, \beta)$ are unitarily equivalent. \square

Now we are ready to prove the main result of this section.

Theorem 5.13. *Let \tilde{H} be a self-adjoint extension of H . Suppose that*

$$C_2 := \sum_{|k-j|>0} \frac{1}{|x_j - x_k|^2} < \infty. \quad (5.55)$$

(i) *Then the part $\tilde{H}E_{\tilde{H}}(C_2, \infty)$ of \tilde{H} is absolutely continuous, i.e.,*

$$\sigma_s(\tilde{H}) \cap (C_2, \infty) = \emptyset. \quad (5.56)$$

Moreover, $\tilde{H}E_{\tilde{H}}(C_2, \infty)$ is unitarily equivalent to the part $-\Delta E_{-\Delta}(C_2, \infty)$ of $-\Delta$.

(ii) *Assume, in addition, that the conditions in Proposition 2.18 are satisfied, i.e., $d_*(X_n) > 0$ and $D^*(X_n) = 0$. Then $\tilde{H}_+ := \tilde{H}E_{\tilde{H}}(\mathbb{R}_+)$ is unitarily equivalent to $H_0 = -\Delta$. In particular, \tilde{H}_+ is purely absolutely continuous, $\tilde{H}_+ = \tilde{H}_+^{ac}$.*

Proof. As in the proof of Proposition 5.5(ii) we decompose the symmetric operator H in a direct sum $H = \widehat{H} \oplus H'$ of a simple symmetric operator \widehat{H} and a self-adjoint operator H' . Next we define a boundary triplet $\widehat{\Pi} = \{\mathcal{H}, \widehat{\Gamma}_0, \widehat{\Gamma}_1\}$ for \widehat{H}^* by setting $\widehat{\Gamma}_j := \Gamma_j \upharpoonright \text{dom}(\widehat{H}^*)$, $j \in \{0, 1\}$, and note that the corresponding Weyl function $\widehat{M}(\cdot)$ coincides with the Weyl function $M(\cdot)$ of Π . Further, any proper extension $\widetilde{H} = H_\Theta$ of H admits a decomposition $H_\Theta = \widehat{H}_\Theta \oplus H'$. In particular, the operator $H_0 = -\Delta$ is decomposed as $H_0 = \widehat{H}_0 \oplus H'$, where $\widehat{H}_0 = \widehat{H}^* \upharpoonright \ker(\widehat{\Gamma}_0) = \widehat{H}_0^*$. Being a part of H_0 , the operator $H' = (H')^*$ is absolutely continuous and $\sigma(H') = \sigma_{ac}(H') \subset \mathbb{R}_+$, because $\sigma(H_0) = \sigma_{ac}(H_0) = \overline{\mathbb{R}_+}$. Therefore, it suffices to prove all assertions for self-adjoint extensions \widehat{H}_Θ of the *simple symmetric operator* \widehat{H} .

(i) To prove (5.56) for any extension of \widehat{H} it suffices to verify the conditions of Lemma 5.12 noting that $\widehat{M}(\cdot) = M(\cdot)$. First we prove that for any $t \in \mathbb{R}_+$ the uniform limit

$$M(t + i0) := u - \lim_{y \downarrow 0} M(t + iy) \cong \left(i\sqrt{t}\delta_{kj} + \frac{e^{i\sqrt{t}|x_k - x_j|} - \delta_{kj}}{|x_k - x_j| + \delta_{kj}} \right)_{j,k=1}^\infty, \quad t \in \mathbb{R}, \quad (5.57)$$

exists, where the symbol $T \cong \mathcal{T}$ means that the operator T has the matrix \mathcal{T} with respect to the standard basis of $l^2(\mathbb{N})$.

Indeed, it follows from (5.12) that for any $\xi, \eta \in l^2(\mathbb{N})$,

$$\langle (M(t + iy) - M(t))\xi, \eta \rangle = (\sqrt{t + iy} - \sqrt{t})\langle \xi, \eta \rangle + \sum'_{j,k \in \mathbb{N}} (e^{-\beta|x_j - x_k|} - 1) \frac{e^{i\alpha|x_j - x_k|}}{|x_j - x_k|} \xi_j \bar{\eta}_k. \quad (5.58)$$

Fix $\varepsilon > 0$. By to the assumption (5.55) there exists $N = N(\varepsilon) \in \mathbb{N}$ such that

$$\sum_{j \geq N} \sum'_{k \in \mathbb{N}} \frac{1}{|x_j - x_k|^2} + \sum_{k \geq N} \sum'_{j \in \mathbb{N}} \frac{1}{|x_j - x_k|^2} < (\varepsilon/2)^2. \quad (5.59)$$

Then

$$\begin{aligned} & \sum_{j \geq N} \sum'_{k \in \mathbb{N}} \frac{1}{|x_j - x_k|} |\xi_j \bar{\eta}_k| + \sum_{k \geq N} \sum'_{j \in \mathbb{N}} \frac{1}{|x_j - x_k|} |\xi_j \bar{\eta}_k| \\ & \leq \left(\sum_{j \geq N} |\xi_j|^2 \right)^{1/2} \left(\sum_{k=1}^\infty |\eta_k|^2 \right)^{1/2} \left(\sum_{j \geq N} \sum'_{k \in \mathbb{N}} \frac{1}{|x_j - x_k|^2} \right)^{1/2} \\ & \quad + \left(\sum_{j \geq N} |\eta_k|^2 \right)^{1/2} \left(\sum_{j=1}^\infty |\xi_k|^2 \right)^{1/2} \left(\sum_{k \geq N} \sum'_{j \in \mathbb{N}} \frac{1}{|x_j - x_k|^2} \right)^{1/2} \\ & \leq 2^{-1} \varepsilon \|\xi\|_{l^2} \cdot \|\eta\|_{l^2}. \end{aligned} \quad (5.60)$$

On the other hand, since $d_*(X) > 0$, we can find $\beta_0 = \beta_0(N)$ such that

$$\sum_{j,k=1}^N \frac{(1 - e^{-\beta|x_j - x_k|})}{|x_j - x_k|} \leq \varepsilon d_*(X)^{-1} \quad \text{for} \quad \beta \in (0, \beta_0). \quad (5.61)$$

Combining (5.58) with (5.60) and (5.61) we get

$$|\langle (M(t + iy) - M(t))\xi, \eta \rangle| \leq \varepsilon (1 + d_*(X)^{-1}) \|\xi\|_{l^2} \cdot \|\eta\|_{l^2}, \quad y \in (0, y_0), \quad (5.62)$$

that is,

$$\|M(t + iy) - M(t)\| \leq \varepsilon(1 + d_*(X)^{-1}) \quad \text{for } y \in (0, y_0). \quad (5.63)$$

Thus, the uniform limit (5.57) exists for any $t \in \mathbb{R}_+$.

Further, it follows from (5.57) that

$$M_I(t) := M_I(t + i0) \cong \sqrt{t} \left(\delta_{kj} + \frac{\sin(\sqrt{t}|x_k - x_j|)}{\sqrt{t}(|x_k - x_j| + \delta_{kj})} \right)_{j,k=1}^{\infty}, \quad t \in \mathbb{R}_+. \quad (5.64)$$

This relation combined with assumption (5.55) yields $0 \in \rho(M_I(t))$ for $t > C_2$. The assertion follows now by applying Lemma 5.12 to the operator \widehat{H} and the interval (C_2, ∞) .

(ii) By (2.12) the function $\Omega_3(t) = \frac{\sin t}{t}$ is in Φ_3 . Hence, by Proposition 2.18, the matrix function $\Omega_3(t\|\cdot\|)$ is strongly X -positively definite for any $t > 0$, i.e., the matrix $\Omega_3(t\|x_j - x_k\|)_{j,k \in \mathbb{N}}$ is positively definite for any $t > 0$. By (5.64) we have

$$M_I(t) := M_I(t + i0) \cong \sqrt{t}\Omega_3(\sqrt{t}\|x_j - x_k\|)_{j,k \in \mathbb{N}}, \quad t \in \mathbb{R}_+.$$

Hence $M_I(t)$ is positively definite for $t \in \mathbb{R}_+$. It remains to apply Lemma 5.12 to the boundary triplet $\widehat{\Pi}$ and the interval \mathbb{R}_+ . \square

Next we present another result on the ac-spectrum of self-adjoint extensions that is based on Corollary 2.24.

Theorem 5.14. *Let \widetilde{H} be an arbitrary self-adjoint extension of H . Assume that*

$$\lim_{p \rightarrow \infty} \left(\sup_{j \in \mathbb{N}} \sum'_{k \in \mathbb{N}} \frac{1}{|x_k - x_j|} \right) = 0 \quad (5.65)$$

and let C_1 be defined by (5.43). Then:

(i) *The part $\widetilde{H}E_{\widetilde{H}}(C_1^2, \infty)$ of \widetilde{H} is absolutely continuous, i.e.*

$$\sigma_s(\widetilde{H}) \cap (C_1^2, \infty) = \emptyset. \quad (5.66)$$

Moreover, $\widetilde{H}E_{\widetilde{H}}(C_1^2, \infty)$ is unitarily equivalent to the part $-\Delta E_{-\Delta}(C_1^2, \infty)$ of $-\Delta$.

(ii) *Assume, in addition, that the conditions of Proposition 2.18 are fulfilled, i.e. $d_*(X_n) > 0$ and $D^*(X_n) = 0$. Then $\widetilde{H}_+ = \widetilde{H}E_{\widetilde{H}}(\mathbb{R}_+)$ is unitarily equivalent to $H_0 = -\Delta$. In particular, \widetilde{H}_+ is purely absolutely continuous, i.e. $\widetilde{H}_+ = \widetilde{H}_+^{ac}$.*

Proof. (i) The proof is similar to that of Theorem 5.13(i). Indeed, by assumption (5.65), for any $\varepsilon > 0$ one can find $N = N(\varepsilon) \in \mathbb{N}$ such that

$$\sup_{j \geq N} \sum'_{k \in \mathbb{N}} \frac{1}{|x_j - x_k|} + \sup_{k \geq N} \sum'_{j \in \mathbb{N}} \frac{1}{|x_j - x_k|} < \varepsilon/2. \quad (5.67)$$

Starting with (5.67) instead of (5.59) and applying Corollary 2.24 we derive

$$\sum_{j \geq N} \sum'_{k \in \mathbb{N}} \frac{1}{|x_j - x_k|} |\xi_j \overline{\eta}_k| + \sum_{k \geq N} \sum'_{j \in \mathbb{N}} \frac{1}{|x_j - x_k|} |\xi_j \overline{\eta}_k| \leq 2^{-1} \varepsilon \|\xi\|_{l^2} \cdot \|\eta\|_{l^2} \quad (5.68)$$

which implies (5.63). That the operator $M_I(\cdot)$ has a bounded inverse if $t > C_1^2$ follows from (5.64) and Proposition 2.27. It remains to apply Lemma 5.12 to the operator \widehat{H} and the interval (C_1^2, ∞) .

(ii) follows by arguing in a similar manner as in the proof of Theorem 5.13(ii). \square

Remark 5.15. (i) The assertions of Theorems 5.13(iii) and 5.14(iii) remains valid if the sequence X satisfies the assumptions of Proposition 2.20(i) instead of Proposition 2.18. The proof of Theorem 5.13(ii) shows that Propositions 2.18 and 2.20(i) guarantee the absence of singular continuous spectrum and of eigenvalues embedded in the ac -spectrum for any self-adjoint extension \tilde{H} of H .

(ii) For sets $X = \{x_j\}_1^m$ of finitely many points a description of the ac -spectrum and the point spectrum of self-adjoint realizations of \mathfrak{L}_3 was obtained by different methods in [4, Theorem 1.1.4] and [21]. For this purpose a connection with radial positive definite functions was exploited for the first time and strong X -positive definiteness of some functions $f \in \Phi_3$ was used in [21].

Remark 5.16. At first glance it seems that Theorem 5.13 might contradict the classical Weyl – von Neumann theorem [31, Theorem X.2.1], [48, Theorem 13.16.1] which states the existence of an additive perturbation $K = K^* \in \mathfrak{S}_2$ such that the operator $H + K$ has a purely point spectrum. In fact, Theorem 5.13 yields explicit examples showing that the analog of the Weyl – von Neumann theorem does not hold for non-additive (singular) compact perturbations. Under the assumptions of Theorem 5.13(ii), for *any* self-adjoint extension \tilde{H} of H , the part $\tilde{H}E_{\tilde{H}}(\mathbb{R}_+)$ is purely absolutely continuous and $\tilde{H}E_{\tilde{H}}(\mathbb{R}_+)$ is unitarily equivalent to $H = -\Delta$. *This shows that both the ac -spectrum $\sigma(H)$ and its multiplicity cannot be eliminated by some perturbations $K_{\tilde{H}} := (\tilde{H} - i)^{-1} - (H_0 - i)^{-1}$ with $\tilde{H} = \tilde{H}^* \in \text{Ext}_H$. That is, the operator $H = -\Delta$ satisfies the property of ac -minimality in the sense of [41]. Moreover, if $K_{\tilde{H}}$ is compact, then $\tilde{H}E_{\tilde{H}}(\mathbb{R}_+)$ is even unitarily equivalent to $H = -\Delta$.* A similar result was obtained for realizations in $L^2(\mathbb{R}_+, \mathcal{H})$ of the differential expression $\mathcal{L} = \frac{d^2}{dx^2} + T$ with unbounded non-negative operator potential $T = T^* \in \mathcal{C}(\mathcal{H})$ in [41]. However, in contrast to our Theorems 5.13, 5.14, the non-negative spectrum of some realizations of \mathcal{L} *might contain a singular part* (see [41]).

Note also that in contrast to the 3D-case one dimensional sparse point interactions (as well as ordinary potentials) may lead to singular spectrum.

Remark 5.17. The absolute continuity of self-adjoint realizations \tilde{H} of H has been studied only for special configurations $X = Y + \Lambda$, where $Y = \{y_j\}_1^N \in \mathbb{R}^3$ is a finite set and $\Lambda = \{\sum_1^3 n_j a_j \in \mathbb{R}^3 : (n_1, n_2, n_3) \in \mathbb{Z}^3\}$ is the Bravais lattice. It was first proved in [23] that in the case $N = 1$ the spectrum of local periodic realizations is absolutely continuous and contains at most two bands (see also [4, Theorems 1.4.5, 1.4.6]). Further development can be found in [3, 5, 28, 29, 30], The most complete result in this direction was obtained in [6]. It was proved in [6] that the spectrum of some (not necessarily local) realizations \tilde{H} is absolutely continuous and has a band structure with a finite number of gaps (for the negative part of the energy axis this result was proved earlier in [5, 28]). In particular, these results confirm the Bethe-Sommerfeld conjecture on the finiteness of bands for the case of periodic perturbations.

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